Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Insight into the direct conversion of methane to methanol on modified ZIF-204 from the perspective of DFT-based calculations

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S1. Linear response method

Linear response method is used to determine the Hubbard U correction for Cu transition metal in ZIF-204.[1] U is calculated through the following equations.

$$\chi_{IJ}^{0} = \frac{\partial N_I^{NSCF}}{\partial V_J} \quad (1)$$

$$\chi_{IJ} = \frac{\partial N_I^{SCF}}{\partial V_J} \quad (2)$$

$$U = \chi_{IJ}^{-1} - \chi_{IJ}^{0\,-1} = \left(\frac{\partial N_I^{SCF}}{\partial V_J}\right)^{-1} - \left(\frac{\partial N_I^{NSCF}}{\partial V_J}\right)^{-1} \quad (3)$$

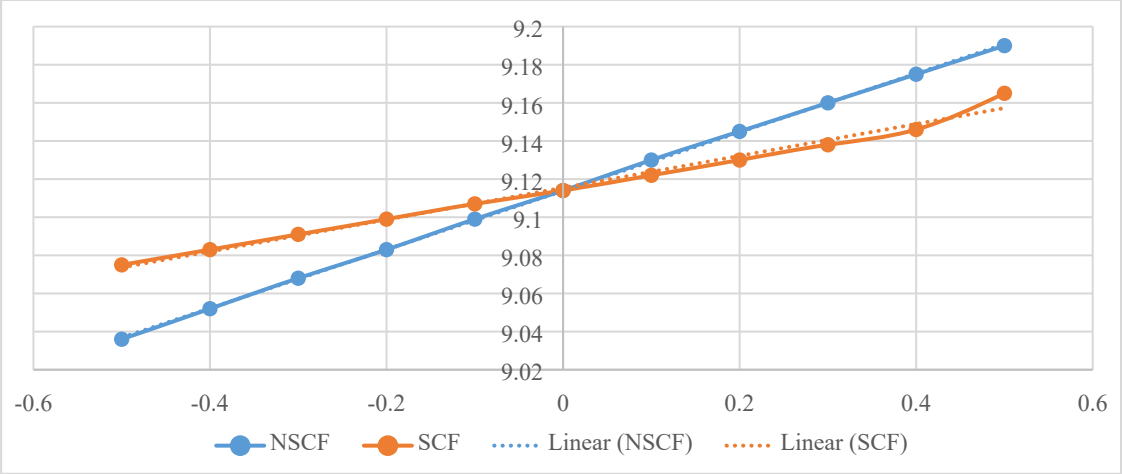

Figure S1. Plot of variation of the numbers of d electrons against potential. The differential of numbers of d electrons vs potential is determined by the tangent of the linear-fitting lines.

Table S1. Variation of the numbers of d electrons against potential, and calculated U derived from linear-fitting values.

V_J (eV)	N_I^{NSCF}	N_I^{SCF}
-0.5	9.036	9.075
-0.4	9.052	9.083
-0.3	9.068	9.091
-0.2	9.083	9.099
-0.1	9.099	9.107
0.0	9.114	9.114
0.1	9.13	9.122
0.2	9.145	9.13

0.3	9.16	9.138
0.4	9.175	9.146
0.5	9.19	9.165
χ_{IJ}	0.154	0.084
$U = {\chi_{IJ}}^{-1} - {\chi_{IJ}^{0}}^{-1} = 5.5$		

S2. Lattice parameters

Table S2. Lattice parameters of pristine ZI calculated by various functionals. Bold numbers with minus (-)/plus (+) signs indicate decrease/increase in percentage (%) between calculated and experimental values.

Functional	a (Å)	b (Å)	c (Å)	β (°)	V (Å^3)
LDA	11.67	12.44	17.10	94.31	2476
	-2.26	**-6.54**	**-3.77**	**-4.11**	**-11.38**
PBE	12.19	13.09	17.55	95.98	2785
	+2.01	**-1.58**	**-1.24**	**-2.41**	**-0.36**
revPBE	11.97	12.71	17.36	93.91	2638
	+0.17	**-4.44**	**-2.36**	**-4.51**	**-5.62**
RPBE	11.82	12.72	17.30	93.67	2597
	-1.09	**-4.36**	**-2.36**	**-4.76**	**-7.08**
PBE-D3	11.96	12.77	17.31	94.30	2636
	+0.17	**-3.98**	**-2.64**	**-4.12**	**-5.65**
PBE-D3-U	11.94	12.76	17.29	94.40	2626
	+0.17	**-4.06**	**-2.70**	**-4.06**	**-6.01**
Exp.[2]	11.95	13.30	17.78	98.35	2795

Lattice parameters are bench-marked on various functionals, for both local and gradient density approximations, i.e., LDA, PBE, PBE-D3, and PBE-D3-U. We found that all applied functionals underestimate lattice parameters and unit-cell volumes. Optimized values from LDA manifest the biggest deviations, smaller than the experimental values, from 2% to 6% for lattice parameters and over 10% for the volume. For PBE functional, the lattice constants a, b, and c are 12.19, 13.09, and 17.55 Å compared to 11.95, 13.30, and 17.78 Å for PBE and experimental values, respectively. This leads to a negligible discrepancy, under 1%, in the volume. Other GGA functionals corrected to PBE like revPBE and RPBE result in differences in unit cell volumes of about 5 to 7 % compared to the experimental value. Including van der Waals corrections, PBE-D3 and PBE-D3-U show a difference less than 4% for lattice constants and 6% for the unit-cell volume. In this work, PBE-D3-U will be employed in all calculations to take into account van der Waals interaction for inert gas methane and the strong-correlated effect for transition metal copper presented in ZI.

S3. Absolute energies and atomic positions

S3.1. CH_4

Energy (eV): -24.07

Simulation cell vectors (Å):

a =	20.000000000	0.000000000	0.000000000
b =	0.000000000	20.000000000	0.000000000
c =	0.000000000	0.000000000	20.000000000

Fractional coordinates:

No.	Element	X	Y	Z
1	C	0.387996282	0.499799460	0.456786962
2	H	0.442797139	0.499799695	0.456798999
3	H	0.369722423	0.465693056	0.417982917
4	H	0.369719238	0.550456461	0.446657079
5	H	0.369714937	0.483251400	0.504973985

S3.2. ZI

Energy (eV): -1121.31

Simulation cell vectors (Å):

a =	11.927633681	0.000000000	0.424723268
b =	0.000000000	12.763023019	0.000000000
c =	-1.937808522	0.000000000	17.183883365

Fractional coordinates:

No.	Element	X	Y	Z
1	Zn	0.701634583	0.532190800	0.194537513
2	Zn	0.298365475	0.467809164	0.805462478
3	Zn	0.798365494	0.032190818	0.305462476
4	Zn	0.201634516	0.967809200	0.694537529
5	Cu	0.034309635	0.665177783	0.446877395
6	Cu	0.965690277	0.334822253	0.553122664
7	Cu	0.465690388	0.165177729	0.053122621
8	Cu	0.534309656	0.834822217	0.946877398
9	Cu	0.500000000	0.500000000	0.500000002
10	Cu	0.000000000	0.000000000	0.000000000
11	N	0.675074332	0.414315565	0.119996465
12	N	0.324925672	0.585684435	0.880003553
13	N	0.824925705	0.914315601	0.380003524
14	N	0.175074320	0.085684444	0.619996454
15	N	0.576717199	0.280690695	0.065392304
16	N	0.423282814	0.719309287	0.934607667
17	N	0.923282880	0.780690713	0.434607691
18	N	0.076717190	0.219309305	0.565392287

19	N	0.586321857	0.521892650	0.272306600
20	N	0.413678192	0.478107350	0.727693351
21	N	0.913678177	0.021892668	0.227693375
22	N	0.086321829	0.978107314	0.772306657
23	N	0.509926333	0.513994618	0.386411451
24	N	0.490073673	0.486005382	0.613588581
25	N	0.990073669	0.013994637	0.113588572
26	N	0.009926288	0.986005382	0.886411426
27	N	0.850651816	0.547877380	0.253264639
28	N	0.149348156	0.452122620	0.746735421
29	N	0.649348144	0.047877362	0.246735364
30	N	0.350651825	0.952122656	0.753264587
31	N	0.976081408	0.603446341	0.347154072
32	N	0.023918632	0.396553659	0.652845932
33	N	0.523918635	0.103446314	0.152845944
34	N	0.476081369	0.896553659	0.847154075
35	N	0.159593371	0.563244315	0.456314740
36	N	0.840406600	0.436755685	0.543685265
37	N	0.340406623	0.063244301	0.043685279
38	N	0.659593350	0.936755685	0.956314688
39	N	0.334521564	0.504245051	0.483024879
40	N	0.665478397	0.495754985	0.516975126
41	N	0.165478434	0.004245034	0.016975112
42	N	0.834521604	0.995754985	0.983024881
43	N	0.089054769	0.721992852	0.548967943
44	N	0.910945291	0.278007183	0.451032062
45	N	0.410945200	0.221992817	0.951032010
46	N	0.589054751	0.778007148	0.048967950
47	N	0.164022799	0.834454583	0.637441875
48	N	0.835977243	0.165545417	0.362558184
49	N	0.335977212	0.334454583	0.862558133
50	N	0.664022797	0.665545417	0.137441818
51	C	0.598854183	0.338489490	0.129874942
52	C	0.401145795	0.661510474	0.870125049
53	C	0.901145854	0.838489526	0.370125046
54	C	0.098854202	0.161510501	0.629874958
55	C	0.703528269	0.404091633	0.044320175
56	C	0.296471738	0.595908403	0.955679857
57	C	0.796471772	0.904091633	0.455679828
58	C	0.203528255	0.095908376	0.544320204
59	C	0.642505747	0.322115721	0.010644066
60	C	0.357494315	0.677884351	0.989355946
61	C	0.857494255	0.822115649	0.489355944
62	C	0.142505716	0.177884279	0.510644061
63	C	0.602164686	0.496442327	0.347846006
64	C	0.397835326	0.503557637	0.652154053
65	C	0.897835357	0.996442350	0.152154010
66	C	0.102164675	0.003557709	0.847845954

67	C	0.477078584	0.558023928	0.261572003
68	C	0.522921484	0.441976072	0.738427948
69	C	0.022921435	0.058023914	0.238427973
70	C	0.977078557	0.941976108	0.761572059
71	C	0.429823861	0.552677047	0.331569225
72	C	0.570176168	0.447322917	0.668430725
73	C	0.070176154	0.052677085	0.168430750
74	C	0.929823873	0.947322953	0.831569282
75	C	0.866521550	0.597496030	0.322028269
76	C	0.133478395	0.402503970	0.677971709
77	C	0.633478410	0.097496030	0.177971734
78	C	0.366521636	0.902503970	0.822028298
79	C	0.956622656	0.521344688	0.232833567
80	C	0.043377365	0.478655348	0.767166438
81	C	0.543377345	0.021344671	0.267166436
82	C	0.456622656	0.978655276	0.732833569
83	C	0.033892304	0.555335425	0.290677813
84	C	0.966107691	0.444664611	0.709322165
85	C	0.466107694	0.055335393	0.209322176
86	C	0.533892270	0.944664611	0.790677842
87	C	0.266885669	0.588612881	0.478964528
88	C	0.733114382	0.411387083	0.521035477
89	C	0.233114338	0.088612917	0.021035461
90	C	0.766885659	0.911387119	0.978964530
91	C	0.158847965	0.456057291	0.445668580
92	C	0.841151966	0.543942673	0.554331425
93	C	0.341152047	0.956057291	0.054331430
94	C	0.658847995	0.043942709	0.945668582
95	C	0.266904464	0.419710431	0.462389507
96	C	0.733095545	0.580289569	0.537610444
97	C	0.233095510	0.919710467	0.037610465
98	C	0.766904508	0.080289560	0.962389618
99	C	0.115548389	0.822724200	0.565055140
100	C	0.884451647	0.177275817	0.434944892
101	C	0.384451594	0.322724200	0.934944921
102	C	0.615548355	0.677275800	0.065055118
103	C	0.122296719	0.666056025	0.615188084
104	C	0.877703238	0.333943939	0.384811948
105	C	0.377703312	0.166056061	0.884811923
106	C	0.622296725	0.833943975	0.115188068
107	C	0.167955772	0.735440165	0.669829620
108	C	0.832044184	0.264559853	0.330170412
109	C	0.332044239	0.235440129	0.830170387
110	C	0.667955776	0.764559835	0.169829591
111	H	0.559707726	0.326194317	0.183757311
112	H	0.440292278	0.673805683	0.816242708
113	H	0.940292312	0.826194317	0.316242678
114	H	0.059707743	0.173805683	0.683757300

115	H	0.764222680	0.455579263	0.020190325
116	H	0.235777293	0.544420701	0.979809646
117	H	0.735777285	0.955579299	0.479809698
118	H	0.264222696	0.044420737	0.520190307
119	H	0.640109242	0.291174667	0.952171027
120	H	0.359890790	0.708825369	0.047828934
121	H	0.859890720	0.791174631	0.547828980
122	H	0.140109213	0.208825333	0.452171079
123	H	0.680118633	0.464797099	0.374320228
124	H	0.319881416	0.535202937	0.625679723
125	H	0.819881324	0.964797079	0.125679761
126	H	0.180118606	0.035202865	0.874320285
127	H	0.442180023	0.585823448	0.205505844
128	H	0.557820017	0.414176517	0.794494160
129	H	0.057820007	0.085823479	0.294494158
130	H	0.942180024	0.914176552	0.705505847
131	H	0.346225423	0.573810292	0.346245357
132	H	0.653774584	0.426189708	0.653754675
133	H	0.153774574	0.073810291	0.153754673
134	H	0.846225377	0.926189708	0.846245332
135	H	0.799029123	0.628383273	0.353926059
136	H	0.200970888	0.371616691	0.646073946
137	H	0.700970921	0.128383300	0.146073957
138	H	0.299029103	0.871616727	0.853926061
139	H	0.969091824	0.479886311	0.179421698
140	H	0.030908120	0.520113689	0.820578320
141	H	0.530908140	0.979886347	0.320578318
142	H	0.469091861	0.020113675	0.679421687
143	H	0.124540520	0.547702786	0.296202956
144	H	0.875459556	0.452297178	0.703797076
145	H	0.375459467	0.047702801	0.203797033
146	H	0.624540485	0.952297250	0.796202931
147	H	0.294669726	0.667698103	0.493242407
148	H	0.705330275	0.332301861	0.506757598
149	H	0.205330270	0.167698121	0.006757573
150	H	0.794669698	0.832301897	0.993242464
151	H	0.083194921	0.414208166	0.425403603
152	H	0.916805020	0.585791869	0.574596402
153	H	0.416805098	0.914208166	0.074596392
154	H	0.583194890	0.085791834	0.925403552
155	H	0.299793904	0.340587747	0.461317760
156	H	0.700206057	0.659412253	0.538682245
157	H	0.200206099	0.840587747	0.038682251
158	H	0.799793916	0.159412244	0.961317817
159	H	0.098628477	0.887058944	0.524782595
160	H	0.901371524	0.112941047	0.475217410
161	H	0.401371512	0.387058980	0.975217358
162	H	0.598628444	0.612941056	0.024782623

163	H	0.111431325	0.581926670	0.618448349
164	H	0.888568666	0.418073330	0.381551656
165	H	0.388568666	0.081926670	0.881551659
166	H	0.611431329	0.918073330	0.118448319
167	H	0.201834873	0.721679362	0.728988504
168	H	0.798165108	0.278320638	0.271011501
169	H	0.298165128	0.221679380	0.771011503
170	H	0.701834855	0.778320638	0.228988515

S3.3. ZI_O

Energy (eV): -1123.91

Simulation cell vectors (Å):

a =	11.936203796	0.033475449	0.361242463
b =	0.036476789	12.757997540	-0.020526162
c =	-2.035129827	-0.033008799	17.281740387

Fractional coordinates:

No.	Element	X	Y	Z
1	Zn	0.696856175	0.533112835	0.196014815
2	Zn	0.304308910	0.463911448	0.802602353
3	Zn	0.804355809	0.034235806	0.303281909
4	Zn	0.196118682	0.966602647	0.695800520
5	Cu	0.031079965	0.663963851	0.448587762
6	Cu	0.965180570	0.335986188	0.552524461
7	Cu	0.465010045	0.163522955	0.053129253
8	Cu	0.534791146	0.833992911	0.946045417
9	Cu	0.502619490	0.519071691	0.502324528
10	Cu	-0.000035887	-0.000322166	0.999541757
11	N	0.670406905	0.414465876	0.122135849
12	N	0.330241395	0.583018492	0.875873436
13	N	0.828839965	0.916757647	0.377557665
14	N	0.170343136	0.083985140	0.621014077
15	N	0.573736249	0.280340060	0.066679028
16	N	0.425948340	0.717177650	0.932052368
17	N	0.922601611	0.781441291	0.434117827
18	N	0.074838901	0.219022630	0.565369054
19	N	0.582319374	0.527743377	0.273368280
20	N	0.418596565	0.467007186	0.724863924
21	N	0.919280091	0.025109687	0.226524982
22	N	0.080990065	0.977607909	0.772513826
23	N	0.509164435	0.522712552	0.387465362
24	N	0.491893479	0.475020069	0.611192586
25	N	0.992662341	0.017021040	0.112518695
26	N	0.007442229	0.984204595	0.886507970
27	N	0.845917011	0.546004696	0.255905841

28	N	0.153983877	0.450222194	0.744444085
29	N	0.654662659	0.047259453	0.244429193
30	N	0.345650040	0.951754038	0.754741014
31	N	0.972122788	0.600717222	0.349841377
32	N	0.025533192	0.396244749	0.651763254
33	N	0.525946574	0.101473504	0.151788572
34	N	0.473691467	0.896418679	0.847467518
35	N	0.158466826	0.564084265	0.458132474
36	N	0.842087204	0.440626933	0.543206597
37	N	0.340537843	0.061462878	0.043185697
38	N	0.659586746	0.935904796	0.955775447
39	N	0.335866189	0.512036166	0.484144601
40	N	0.668806832	0.504670340	0.518426239
41	N	0.165565078	0.003010483	0.015911699
42	N	0.834360362	0.994916504	0.983130932
43	N	0.085063500	0.720095031	0.550764038
44	N	0.909609522	0.280200003	0.450924790
45	N	0.409946402	0.219350892	0.950999348
46	N	0.590007926	0.778195186	0.048266394
47	N	0.159189038	0.832860906	0.639332536
48	N	0.839188107	0.167913783	0.360790879
49	N	0.338579179	0.331337091	0.861007650
50	N	0.662317449	0.666215837	0.138048183
51	O	0.499657552	0.665463626	0.530397556
52	C	0.593914540	0.339058452	0.130772783
53	C	0.406074078	0.659124659	0.867580948
54	C	0.904547702	0.839543103	0.369769886
55	C	0.094274484	0.160670597	0.629499044
56	C	0.701189816	0.402909471	0.047734403
57	C	0.299511648	0.593401240	0.950374748
58	C	0.796319473	0.907139807	0.451558146
59	C	0.201705545	0.094248158	0.546752089
60	C	0.641200579	0.320602215	0.013543596
61	C	0.358904925	0.675759858	0.985006679
62	C	0.854579926	0.824104704	0.486461104
63	C	0.142450902	0.177182838	0.512394503
64	C	0.597783734	0.498004491	0.347649649
65	C	0.404566476	0.501539597	0.651802170
66	C	0.901978555	0.998818459	0.151510138
67	C	0.098185185	0.002987377	0.847698194
68	C	0.477500085	0.575191553	0.265163173
69	C	0.521945914	0.416657956	0.731828231
70	C	0.027928319	0.062655060	0.236475555
71	C	0.972364082	0.940030574	0.762263789
72	C	0.432474086	0.571668754	0.335302515
73	C	0.567648521	0.422781962	0.661943888
74	C	0.073336046	0.057169526	0.166538735
75	C	0.926876589	0.944582245	0.832199930

76	C	0.862493025	0.597162066	0.323825548
77	C	0.135886352	0.401973885	0.675527131
78	C	0.635997684	0.098178418	0.176812969
79	C	0.363609492	0.901409868	0.822688090
80	C	0.951394696	0.515852407	0.237053956
81	C	0.048847495	0.475932477	0.766442196
82	C	0.550179140	0.016863725	0.264248738
83	C	0.450646362	0.979705048	0.734458673
84	C	0.029191604	0.549365131	0.294909441
85	C	0.969635651	0.442892761	0.709329523
86	C	0.470870216	0.050090296	0.207178663
87	C	0.529510271	0.945863443	0.791584661
88	C	0.264744346	0.594053919	0.479276827
89	C	0.734297529	0.418599941	0.518949043
90	C	0.233018221	0.087203903	0.020435952
91	C	0.767186957	0.910516419	0.978608382
92	C	0.162303373	0.456477123	0.449412728
93	C	0.845091808	0.546882706	0.558861602
94	C	0.341639563	0.954220937	0.053425084
95	C	0.658132230	0.043146512	0.945481235
96	C	0.272260134	0.424188415	0.465866223
97	C	0.737810231	0.586357181	0.543283707
98	C	0.233524499	0.918199283	0.036334189
99	C	0.766117727	0.079475877	0.962540254
100	C	0.108727311	0.821170770	0.567616056
101	C	0.885488161	0.179273514	0.433622405
102	C	0.385990137	0.320313733	0.933619845
103	C	0.613424225	0.677154799	0.065810783
104	C	0.122627127	0.663796261	0.615751491
105	C	0.876974754	0.336685862	0.385059514
106	C	0.375940978	0.162461847	0.885425941
107	C	0.625902509	0.835228835	0.113407955
108	C	0.167665619	0.733416186	0.670495862
109	C	0.834120702	0.267304035	0.329396220
110	C	0.332487742	0.231545353	0.829853017
111	C	0.669914847	0.766190318	0.168844383
112	H	0.553312748	0.327564084	0.183508036
113	H	0.446377312	0.671720778	0.814843495
114	H	0.946154785	0.826314795	0.317530586
115	H	0.053389453	0.173288769	0.682103074
116	H	0.762588763	0.453835466	0.024763389
117	H	0.238508765	0.541809377	0.973087327
118	H	0.734446658	0.959257970	0.473609691
119	H	0.263035074	0.042147562	0.524008987
120	H	0.640613695	0.288747604	0.955687339
121	H	0.359308090	0.707007442	0.043029579
122	H	0.853396899	0.793034551	0.544226799
123	H	0.142664925	0.208656886	0.454631713

124	H	0.673118196	0.458777257	0.372402666
125	H	0.332349194	0.546528794	0.628424633
126	H	0.824056291	0.966091289	0.125625274
127	H	0.176130337	0.035414887	0.873790040
128	H	0.443975643	0.608681696	0.210657150
129	H	0.553562428	0.378464353	0.785020892
130	H	0.063880258	0.091336140	0.291964439
131	H	0.936549177	0.911819838	0.706602277
132	H	0.352672945	0.600967891	0.351748332
133	H	0.646806057	0.392823492	0.644789912
134	H	0.156054295	0.079125295	0.151410911
135	H	0.844171704	0.922292963	0.847145032
136	H	0.795563515	0.630954292	0.354456066
137	H	0.202198946	0.372031242	0.642512899
138	H	0.701748679	0.131950366	0.145624616
139	H	0.297339956	0.869328417	0.854263512
140	H	0.963247860	0.472316136	0.184678153
141	H	0.038189417	0.516339987	0.820307498
142	H	0.540099378	0.973286518	0.316602836
143	H	0.461488275	0.021589966	0.681504940
144	H	0.119687591	0.539434705	0.301462648
145	H	0.878874297	0.450458249	0.704918224
146	H	0.380528104	0.039794156	0.201475629
147	H	0.620090984	0.954202492	0.796878564
148	H	0.290377897	0.674227577	0.491908363
149	H	0.705060585	0.341213101	0.500983562
150	H	0.204977303	0.166447070	0.006437250
151	H	0.795487820	0.831359873	0.992648124
152	H	0.088060802	0.411627331	0.430440722
153	H	0.921598643	0.585711253	0.581255501
154	H	0.417636505	0.912117102	0.073532011
155	H	0.582055322	0.085006331	0.925224751
156	H	0.309075791	0.346315916	0.466135425
157	H	0.704760238	0.665339821	0.547560476
158	H	0.200713530	0.839165838	0.037041562
159	H	0.798699421	0.158588203	0.961742180
160	H	0.088675793	0.885738404	0.528303591
161	H	0.902711762	0.114607641	0.473319352
162	H	0.404089165	0.385298989	0.973088037
163	H	0.594168793	0.612061050	0.026636831
164	H	0.115255966	0.579294125	0.618053477
165	H	0.886351851	0.420993881	0.382891349
166	H	0.384839627	0.077965626	0.883253911
167	H	0.617642621	0.919793911	0.115435225
168	H	0.204141902	0.719493291	0.728904741
169	H	0.801390380	0.281431018	0.270177984
170	H	0.298701574	0.217027494	0.770873000
171	H	0.704798892	0.780841102	0.227559995

S3.4. CH_4/ZI

Energy (eV): -1145.62

Simulation cell vectors (Å):

a =	11.900190288	0.016974350	-0.000918454
b =	0.015221667	12.739447978	-0.005982152
c =	-1.322813592	-0.013588514	17.316710877

Fractional coordinates:

No	Elements	X	Y	Z
1	Zn	0.675345033	0.531306684	0.206008035
2	Zn	0.276106339	0.462858798	0.815337722
3	Zn	0.777792073	0.031916894	0.315186473
4	Zn	0.176002495	0.963135844	0.705768406
5	Cu	0.007661176	0.662022113	0.458590760
6	Cu	0.942275062	0.332498570	0.563570929
7	Cu	0.443157743	0.162223635	0.064035581
8	Cu	0.510966149	0.831824695	0.957043648
9	Cu	0.475490847	0.499366422	0.510457615
10	Cu	-0.022961131	-0.003354334	0.010642663
11	N	0.650041859	0.412823732	0.132027023
12	N	0.303049504	0.581212228	0.889471478
13	N	0.803163202	0.914766939	0.390227904
14	N	0.149190292	0.080764611	0.631256451
15	N	0.553026586	0.278527681	0.077146812
16	N	0.401281987	0.714855557	0.944347030
17	N	0.898228672	0.779403359	0.445599825
18	N	0.052475713	0.215374137	0.576099943
19	N	0.559134677	0.523762931	0.283236618
20	N	0.390880286	0.472021925	0.737206270
21	N	0.893767180	0.021290773	0.238011325
22	N	0.060126411	0.971581704	0.783288557
23	N	0.484345491	0.516631581	0.397512449
24	N	0.466413775	0.481438031	0.623273364
25	N	0.968813854	0.012832178	0.123811931
26	N	-0.014344209	-0.021367742	0.897719764
27	N	0.824283346	0.545679800	0.265201395
28	N	0.126222412	0.447600204	0.757229034
29	N	0.628137199	0.045484481	0.256719505
30	N	0.325635776	0.948420838	0.764259891
31	N	0.949949448	0.600917211	0.358816327
32	N	0.000263258	0.393256396	0.663431050
33	N	0.501258288	0.100344686	0.163597534
34	N	0.452010212	0.893256680	0.857603787
35	N	0.133232523	0.559895551	0.467898200

36	N	0.816735928	0.435088283	0.554287416
37	N	0.317924147	0.060440504	0.054118575
38	N	0.635821886	0.934568698	0.966734336
39	N	0.309427176	0.502446218	0.494135258
40	N	0.641620107	0.494869190	0.526678961
41	N	0.142939962	0.001537416	0.026268473
42	N	0.811030206	0.993559236	-0.005472076
43	N	0.062093652	0.717744735	0.560886717
44	N	0.888488534	0.277275315	0.461135883
45	N	0.389483283	0.218004390	0.961595158
46	N	0.565380583	0.776023986	0.059181821
47	N	0.139650264	0.829519395	0.648715594
48	N	0.814304254	0.165604936	0.372010325
49	N	0.314551459	0.329681678	0.872643127
50	N	0.639244839	0.664493131	0.148510504
51	C	0.573293167	0.337141895	0.141238574
52	C	0.379473986	0.657121279	0.879968055
53	C	0.878040140	0.837045507	0.381077292
54	C	0.073025071	0.157412329	0.640415195
55	C	0.680866656	0.401669472	0.057237936
56	C	0.274096148	0.591273623	0.964767883
57	C	0.773547910	0.906103165	0.465421450
58	C	0.179301760	0.090526325	0.556243053
59	C	0.620683093	0.319216450	0.023425904
60	C	0.335090635	0.673207293	-0.001367462
61	C	0.832495184	0.822959588	0.499570267
62	C	0.119340919	0.173183500	0.522243023
63	C	0.575143953	0.496086909	0.358017349
64	C	0.375030129	0.500459779	0.662578776
65	C	0.877157565	0.994998746	0.162973593
66	C	0.076109262	-0.000590456	0.858075510
67	C	0.451286209	0.564761715	0.274067414
68	C	0.499151157	0.432120045	0.746443609
69	C	0.002962333	0.058425151	0.247759358
70	C	0.952640676	0.930228681	0.774282874
71	C	0.404978580	0.559829097	0.344188909
72	C	0.545938037	0.438447333	0.676564216
73	C	0.049398764	0.052705354	0.177705615
74	C	0.906536130	0.935086578	0.844493283
75	C	0.840203855	0.596359556	0.333316624
76	C	0.110124025	0.398349347	0.688556669
77	C	0.611192901	0.096044629	0.188712849
78	C	0.342017755	0.899098115	0.832817558
79	C	0.930400536	0.516942744	0.245594758
80	C	0.020017102	0.474781985	0.777615695
81	C	0.522469062	0.016417079	0.276721463
82	C	0.431719863	0.974909235	0.743598295
83	C	0.007808859	0.550760889	0.303270073

84	C	0.942405199	0.441577088	0.719827851
85	C	0.444302187	0.049996462	0.219331919
86	C	0.509574886	0.941243958	0.801129166
87	C	0.240386186	0.586264713	0.490731637
88	C	0.709438531	0.410173241	0.530642937
89	C	0.210449884	0.086098996	0.031264519
90	C	0.742988029	0.909336296	0.990866455
91	C	0.134013559	0.452693875	0.456430472
92	C	0.817265238	0.542348295	0.565746910
93	C	0.318998654	0.952935160	0.063839203
94	C	0.635581192	0.041635108	0.954749577
95	C	0.242915588	0.417269642	0.472898248
96	C	0.709108492	0.579164586	0.548449573
97	C	0.210846080	0.916634703	0.046423277
98	C	0.743805043	0.077943162	0.972066669
99	C	0.089176115	0.818442210	0.577136865
100	C	0.863284991	0.176423274	0.444037708
101	C	0.363562165	0.318824385	0.944687101
102	C	0.591962380	0.675325727	0.076035522
103	C	0.097183636	0.661098681	0.626193300
104	C	0.853690183	0.334321048	0.395969962
105	C	0.355236823	0.160983705	0.896272729
106	C	0.597417570	0.832913011	0.124984591
107	C	0.144427323	0.730072038	0.680450065
108	C	0.808588054	0.265419102	0.340910317
109	C	0.309648808	0.229880207	0.841341764
110	C	0.642312725	0.764078063	0.180196803
111	C	0.468714202	0.787716025	0.520596586
112	H	0.532383337	0.325507498	0.194312767
113	H	0.419058786	0.669518710	0.826464544
114	H	0.917630690	0.823184584	0.327712818
115	H	0.032750892	0.170214057	0.693647443
116	H	0.742543843	0.452815926	0.033794163
117	H	0.213082433	0.539729620	0.988521627
118	H	0.713767845	0.959581187	0.488904989
119	H	0.240595624	0.038519743	0.532856089
120	H	0.620002924	0.287534482	0.965454203
121	H	0.337045417	0.704140786	0.056883700
122	H	0.833500986	0.792515045	0.557852434
123	H	0.118481067	0.204197237	0.464117867
124	H	0.652315821	0.460986233	0.383353622
125	H	0.297689404	0.535192493	0.637210459
126	H	0.799031574	0.962569556	0.137210706
127	H	0.152974724	0.034913299	0.883297324
128	H	0.416612402	0.595320433	0.218964458
129	H	0.533860080	0.401366321	0.801478050
130	H	0.038502793	0.087111735	0.303212275
131	H	0.918118564	0.899428901	0.719205450

132	H	0.322475972	0.583990450	0.359945703
133	H	0.628807349	0.415177497	0.660969338
134	H	0.132724585	0.074411041	0.162390856
135	H	0.824354802	0.910534898	0.860340330
136	H	0.772643395	0.628912549	0.364533081
137	H	0.177731561	0.367141679	0.656712503
138	H	0.678209342	0.128825012	0.157302731
139	H	0.274597259	0.868274427	0.864814216
140	H	0.942886756	0.474091183	0.192884704
141	H	0.007618605	0.516280484	0.830907064
142	H	0.510835695	0.973535276	0.329447139
143	H	0.443936524	0.015968953	0.690203710
144	H	0.098603089	0.541588457	0.309310017
145	H	0.851515470	0.449986531	0.714229391
146	H	0.353593118	0.040512544	0.213596322
147	H	0.600507106	0.948900057	0.806405489
148	H	0.267092148	0.665559961	0.505546614
149	H	0.681798153	0.331169604	0.515608374
150	H	0.182545416	0.165520394	0.017557499
151	H	0.770390138	0.830360750	0.006457635
152	H	0.058855852	0.410147868	0.435834271
153	H	0.892791012	0.583933721	0.586881270
154	H	0.394799485	0.910846644	0.084136009
155	H	0.560243627	0.083554703	0.933301949
156	H	0.277171844	0.338406562	0.471263973
157	H	0.675854446	0.658388840	0.549923749
158	H	0.178012587	0.837339815	0.046709580
159	H	0.777093269	0.156963704	0.970124930
160	H	0.071211637	0.883226455	0.537547779
161	H	0.881546870	0.111346457	0.483314931
162	H	0.381265536	0.383891943	0.984110816
163	H	0.575770212	0.610369994	0.036268538
164	H	0.086537383	0.576782670	0.629085437
165	H	0.863205643	0.418800333	0.393720912
166	H	0.365287471	0.076508499	0.893800535
167	H	0.586645945	0.917302898	0.127535422
168	H	0.179846624	0.715736261	0.738948897
169	H	0.773908287	0.280077323	0.282284300
170	H	0.275218617	0.215264117	0.782647055
171	H	0.675192141	0.778597627	0.239239653
172	H	0.466878285	0.730979445	0.472913272
173	H	0.545345878	0.835168733	0.519788532
174	H	0.468427864	0.746541402	0.576006761
175	H	0.394369977	0.838869359	0.513345699

S3.5. CH_4_ads_s/ZI_O

Energy (eV): -1148.28

Simulation cell vectors (Å):

a =	11.795000076	0.000000000	0.000000000
b =	-0.015655182	12.813990566	0.000000000
c =	-1.452735456	0.007372060	17.409491129

Fractional coordinates:

No.	Element	X	Y	Z
1	Zn	0.677774248	0.527659293	0.208497853
2	Zn	0.286902094	0.455180836	0.811778353
3	Zn	0.784246682	0.037171144	0.317557971
4	Zn	0.172942737	0.966857681	0.709547189
5	Cu	0.016257593	0.670241211	0.457780077
6	Cu	0.940629823	0.337087823	0.565166146
7	Cu	0.448276573	0.161273374	0.064921753
8	Cu	0.509392981	0.828207962	0.960331994
9	Cu	0.482396292	0.514192378	0.511729883
10	Cu	0.978516122	0.995225153	0.013859000
11	N	0.656757839	0.411107849	0.132816593
12	N	0.313362028	0.574470865	0.883584553
13	N	0.811266334	0.921719869	0.392846021
14	N	0.146341626	0.085728859	0.636220594
15	N	0.560356115	0.276818656	0.077148032
16	N	0.402803552	0.709972371	0.942403735
17	N	0.904087637	0.784378429	0.446217699
18	N	0.049770184	0.219296785	0.579920493
19	N	0.564852031	0.497827128	0.285390043
20	N	0.397798339	0.443081585	0.731432260
21	N	0.899742518	0.026211066	0.240319646
22	N	0.056742685	0.974450829	0.786631552
23	N	0.489902348	0.482171284	0.398384787
24	N	0.465222427	0.449397147	0.615826735
25	N	0.972375659	0.015381564	0.126223572
26	N	0.984076357	0.979686571	0.900979461
27	N	0.828506703	0.550271091	0.266735279
28	N	0.133018097	0.448144836	0.755261304
29	N	0.633173922	0.049649962	0.259036413
30	N	0.323579475	0.950653416	0.769210890
31	N	0.955790425	0.607822475	0.359359876
32	N	0.001546674	0.397384732	0.663241915
33	N	0.506456034	0.102170759	0.164608835
34	N	0.450811306	0.892521364	0.861664290
35	N	0.145611376	0.571479766	0.464998425
36	N	0.816758542	0.442213694	0.554747054
37	N	0.322319668	0.058748645	0.056414099
38	N	0.634435524	0.930585946	0.972426312

39	N	0.321408395	0.516931124	0.495831300
40	N	0.643503967	0.508507114	0.531157915
41	N	0.145839398	0.998134018	0.029141512
42	N	0.811229567	0.989931964	0.999559328
43	N	0.072032614	0.723528981	0.559857592
44	N	0.889098896	0.283172480	0.463125320
45	N	0.391756193	0.215812959	0.963181535
46	N	0.561503799	0.771544605	0.063086405
47	N	0.140210072	0.834452240	0.651041458
48	N	0.820601107	0.171218279	0.372890384
49	N	0.315502678	0.324892715	0.873378046
50	N	0.632268432	0.659906454	0.153227275
51	N	0.481848910	0.664151624	0.533560585
52	O	0.581998062	0.333198200	0.141725233
53	C	0.389247500	0.652194666	0.877905073
54	C	0.885276073	0.843879822	0.382886383
55	C	0.067650722	0.160496844	0.643694885
56	C	0.684867597	0.403658094	0.057713154
57	C	0.275781237	0.583516806	0.956222684
58	C	0.780752912	0.911117086	0.467211368
59	C	0.181208121	0.097960079	0.563081703
60	C	0.625175268	0.321193759	0.023411044
61	C	0.331333391	0.666751928	0.992489676
62	C	0.838250827	0.826687816	0.500102372
63	C	0.121378827	0.179964041	0.528340937
64	C	0.585984400	0.486134597	0.361741383
65	C	0.391547155	0.490420431	0.662327194
66	C	0.882493827	0.994919080	0.166740666
67	C	0.074958186	0.999963685	0.861365794
68	C	0.447704472	0.501673684	0.272108461
69	C	0.480886545	0.367429633	0.728773296
70	C	0.007467576	0.069468067	0.247556022
71	C	0.947261780	0.935183396	0.777624578
72	C	0.401558256	0.492057550	0.341532954
73	C	0.522971979	0.371890899	0.657521038
74	C	0.052453764	0.062291451	0.177558198
75	C	0.902308519	0.938909534	0.847776824
76	C	0.844903047	0.602713810	0.333634566
77	C	0.113365643	0.401635926	0.686383778
78	C	0.617406255	0.094921203	0.189343578
79	C	0.339912884	0.898074041	0.836103357
80	C	0.935537637	0.520973659	0.248215596
81	C	0.027285154	0.474404979	0.777927458
82	C	0.525652793	0.027574877	0.280538040
83	C	0.430672674	0.979427386	0.750448731
84	C	0.013906384	0.556247214	0.305246568
85	C	0.946151669	0.443312153	0.721193438
86	C	0.447518386	0.059586761	0.222272266

87	C	0.509020924	0.943894986	0.807364721
88	C	0.254130068	0.600703459	0.483134844
89	C	0.707828243	0.421733526	0.530029853
90	C	0.213931946	0.082489517	0.031873644
91	C	0.743108257	0.905618451	0.995234142
92	C	0.144331561	0.463606310	0.466280040
93	C	0.821307772	0.547527587	0.572093114
94	C	0.323340846	0.952665358	0.069920477
95	C	0.633238589	0.037321526	0.962003548
96	C	0.253653603	0.429364582	0.485870482
97	C	0.713813529	0.588766272	0.557559473
98	C	0.214316032	0.915318949	0.052890854
99	C	0.742477915	0.073952815	0.979059071
100	C	0.091643689	0.824204599	0.578980455
101	C	0.864566997	0.182674660	0.445940321
102	C	0.367002855	0.315854447	0.944809530
103	C	0.584582078	0.670967945	0.080868742
104	C	0.110659741	0.665848882	0.623668365
105	C	0.859346858	0.339176806	0.396875102
106	C	0.354187335	0.157531211	0.899507032
107	C	0.596482191	0.828163272	0.128221678
108	C	0.152017700	0.734317860	0.679999861
109	C	0.817573380	0.270045948	0.341151711
110	C	0.307620000	0.224735595	0.844072586
111	C	0.639522366	0.759386597	0.183763748
112	C	0.523555167	0.762516380	0.378013953
113	H	0.543541634	0.318262677	0.194958535
114	H	0.434082210	0.666500785	0.827102658
115	H	0.925383515	0.831369276	0.329950115
116	H	0.023928030	0.171550653	0.695352931
117	H	0.744477926	0.457165352	0.034350157
118	H	0.213119637	0.530385271	0.976489726
119	H	0.720001742	0.963107957	0.490743999
120	H	0.245122975	0.047695461	0.541292061
121	H	0.623036334	0.291962305	0.965102050
122	H	0.326514263	0.697431618	0.049913097
123	H	0.837668908	0.794228351	0.557326613
124	H	0.123471232	0.212108285	0.471045522
125	H	0.670702163	0.480266743	0.390227682
126	H	0.333666785	0.553814847	0.645846630
127	H	0.805093127	0.957286884	0.142999604
128	H	0.153790506	0.033419364	0.886562845
129	H	0.406372237	0.511494435	0.214707917
130	H	0.502083310	0.315278484	0.776765464
131	H	0.043046742	0.102917567	0.301342452
132	H	0.910535095	0.906541964	0.722594392
133	H	0.313338747	0.491095754	0.354245270
134	H	0.589202372	0.326079736	0.634251750

135	H	0.134509715	0.087224254	0.160679749
136	H	0.819285767	0.915174899	0.863610177
137	H	0.777105850	0.636985144	0.363599712
138	H	0.179831852	0.371755457	0.653068534
139	H	0.685908391	0.122076817	0.156627431
140	H	0.271779223	0.864666415	0.866317785
141	H	0.947837448	0.476827067	0.196598214
142	H	0.017620325	0.513670134	0.831990017
143	H	0.512804846	0.990202114	0.334827459
144	H	0.443184132	0.023149013	0.698629258
145	H	0.105576256	0.548122416	0.311593016
146	H	0.854383378	0.451357391	0.717384314
147	H	0.355520505	0.053878730	0.217203724
148	H	0.600712829	0.952459115	0.813561154
149	H	0.285402572	0.680026302	0.488789205
150	H	0.676679016	0.346208892	0.509666304
151	H	0.185617907	0.160461544	0.015350018
152	H	0.771478012	0.826857058	0.009268431
153	H	0.067088567	0.419336538	0.451782696
154	H	0.899430551	0.584894875	0.594831909
155	H	0.399524978	0.912031866	0.092250731
156	H	0.556629787	0.078703365	0.941452098
157	H	0.287598055	0.351234341	0.493756446
158	H	0.679975828	0.666579820	0.563328072
159	H	0.181127436	0.836644691	0.056143324
160	H	0.775572512	0.152884669	0.978257873
161	H	0.069965480	0.889513948	0.541023557
162	H	0.879866487	0.118436862	0.485953787
163	H	0.387440967	0.381572813	0.982637658
164	H	0.566284135	0.606262677	0.041701596
165	H	0.106269801	0.581341817	0.624320373
166	H	0.870076302	0.423060378	0.394316674
167	H	0.362807328	0.073392849	0.898477782
168	H	0.588959940	0.912393558	0.130271102
169	H	0.187853639	0.719119808	0.738169603
170	H	0.786748309	0.283885653	0.281763825
171	H	0.270772171	0.208872762	0.786249330
172	H	0.673622387	0.774076159	0.242349314
173	H	0.601273404	0.809890479	0.382403859
174	H	0.503561439	0.739436841	0.436278380
175	H	0.535987444	0.692347094	0.343981085
176	H	0.452648482	0.807572149	0.350227523

S3.6. CH_4_ads_t/ZI_O

Energy (eV): -1148.20

Simulation cell vectors (Å):

a =	11.794765740	-0.019322595	-0.008837918
b =	0.005666084	12.813668225	0.007222792
c =	-1.439626879	-0.000055754	17.410206455

Fractional coordinates:

No.	Elements	X	Y	Z
1	Zn	0.678217064	0.531074904	0.207425406
2	Zn	0.287356457	0.455300122	0.811243439
3	Zn	0.782593286	0.034614978	0.316326426
4	Zn	0.171887023	0.969192871	0.707856811
5	Cu	0.012212592	0.667727285	0.460282196
6	Cu	0.940069027	0.337694785	0.563454311
7	Cu	0.444416835	0.162709304	0.065934576
8	Cu	0.508653736	0.830630567	0.958136775
9	Cu	0.479554106	0.512808533	0.511638076
10	Cu	0.976380107	0.996641025	0.011928596
11	N	0.653321353	0.413198596	0.133507768
12	N	0.313903694	0.575507105	0.882407189
13	N	0.806629744	0.917466172	0.390358642
14	N	0.146320318	0.087176668	0.633975546
15	N	0.555034687	0.279515429	0.078533017
16	N	0.402771746	0.711914878	0.940411022
17	N	0.900692380	0.782336514	0.446078310
18	N	0.049552631	0.220614059	0.577753925
19	N	0.563095793	0.515213099	0.284861659
20	N	0.398964359	0.441216777	0.731557583
21	N	0.897594739	0.024359488	0.238776590
22	N	0.055240810	0.978120883	0.784695981
23	N	0.486725531	0.502918413	0.397357433
24	N	0.463933133	0.445104244	0.615146988
25	N	0.970233145	0.015103235	0.124597651
26	N	0.982099393	0.982078507	0.898926437
27	N	0.828520082	0.550325939	0.266741656
28	N	0.134157971	0.448275183	0.753688941
29	N	0.631220862	0.047662384	0.258091151
30	N	0.322694107	0.952782989	0.767094355
31	N	0.954475309	0.605382098	0.361053238
32	N	0.002475612	0.398670247	0.661348219
33	N	0.503195501	0.102661841	0.165267334
34	N	0.449970568	0.894613873	0.859476257
35	N	0.141567466	0.568881226	0.469672887
36	N	0.815366218	0.442078812	0.553495787
37	N	0.319307360	0.059435652	0.056650448
38	N	0.632342678	0.934343100	0.970567112
39	N	0.318769875	0.514840702	0.495773441

40	N	0.641011110	0.506235606	0.530086547
41	N	0.143390425	-0.001327130	0.027481266
42	N	0.809436785	0.993232281	0.997553008
43	N	0.065332836	0.722978535	0.562287445
44	N	0.886455672	0.281705903	0.462017238
45	N	0.388679334	0.216328632	0.963729619
46	N	0.561878375	0.773721787	0.060643331
47	N	0.136211627	0.835884444	0.651223458
48	N	0.819402590	0.168681510	0.371955447
49	N	0.313408562	0.325319647	0.873507974
50	N	0.635106019	0.662789673	0.150446032
51	N	0.476483261	0.657459572	0.548634372
52	O	0.576557169	0.337045681	0.142572436
53	C	0.389702430	0.653236511	0.876335142
54	C	0.883887834	0.841637993	0.382509895
55	C	0.067905989	0.162136652	0.641614953
56	C	0.682748209	0.403505974	0.058829710
57	C	0.275875959	0.585561890	0.954860841
58	C	0.771662198	0.905570482	0.463483437
59	C	0.180517758	0.098933595	0.560595674
60	C	0.621854266	0.321460894	0.024959100
61	C	0.331072631	0.669359881	0.990628205
62	C	0.830098867	0.822627660	0.497876735
63	C	0.120460193	0.180836813	0.525932300
64	C	0.579823399	0.486840397	0.359107712
65	C	0.392040285	0.487840361	0.662195023
66	C	0.879822853	0.995163854	0.164741547
67	C	0.073602546	0.001659080	0.859759730
68	C	0.452762046	0.552072292	0.274992681
69	C	0.480720672	0.364403487	0.728588029
70	C	0.006197736	0.065648940	0.246700042
71	C	0.944922466	0.940957501	0.774948659
72	C	0.405577840	0.544443767	0.344113819
73	C	0.521392341	0.367503642	0.656808660
74	C	0.051151780	0.059465436	0.176657583
75	C	0.899668211	0.943877755	0.845040733
76	C	0.843737492	0.599385106	0.335105642
77	C	0.114393364	0.402747165	0.684411232
78	C	0.614321847	0.096806774	0.189923638
79	C	0.339225792	0.898867311	0.833380767
80	C	0.936163039	0.524282779	0.247503843
81	C	0.028481326	0.473992613	0.776695457
82	C	0.524331495	0.021233024	0.278656957
83	C	0.429522677	0.983896772	0.749288022
84	C	0.013733645	0.557979527	0.305563511
85	C	0.947246695	0.443618146	0.719782815
86	C	0.445379818	0.054903484	0.221417838
87	C	0.507889629	0.948381773	0.806194331

88	C	0.248956929	0.597831934	0.492186604
89	C	0.706547131	0.420354821	0.529041234
90	C	0.211096500	0.083256526	0.031712844
91	C	0.741205130	0.909029598	0.992517104
92	C	0.143757080	0.462047343	0.458967016
93	C	0.818388749	0.547373976	0.570793085
94	C	0.320623677	0.953024979	0.068774064
95	C	0.631138656	0.041276453	0.961466680
96	C	0.253934510	0.428145878	0.475291636
97	C	0.710197601	0.587283430	0.556172747
98	C	0.211890579	0.915607727	0.050636047
99	C	0.740637910	0.077599268	0.978383178
100	C	0.086236859	0.824047089	0.579674441
101	C	0.862252724	0.181048607	0.445226426
102	C	0.364527581	0.316373328	0.945035483
103	C	0.586888779	0.673418202	0.078178308
104	C	0.104175318	0.666873816	0.626833429
105	C	0.857751982	0.336976271	0.395272467
106	C	0.351015035	0.157886394	0.900114171
107	C	0.596042646	0.830555189	0.125822082
108	C	0.147296141	0.736536348	0.681738053
109	C	0.816889144	0.267184468	0.339678410
110	C	0.305028420	0.225046468	0.844437543
111	C	0.640468367	0.762198012	0.181216708
112	C	0.413055337	0.902036152	0.529973250
113	H	0.536694474	0.324167635	0.195575458
114	H	0.434762283	0.666917407	0.825539408
115	H	0.927520075	0.830353774	0.330847637
116	H	0.024744303	0.173502541	0.693476814
117	H	0.743990119	0.455335793	0.035442745
118	H	0.213305103	0.532571097	0.975424765
119	H	0.707669262	0.955766030	0.485262628
120	H	0.244236816	0.048633161	0.538686964
121	H	0.620108409	0.290978738	0.967019889
122	H	0.325937676	0.700797382	0.047808562
123	H	0.827339172	0.790077721	0.554915940
124	H	0.122070588	0.212741401	0.468552323
125	H	0.659020422	0.454626180	0.384653709
126	H	0.335604276	0.552336255	0.645918978
127	H	0.801698760	0.959356739	0.140448657
128	H	0.152990346	0.033202427	0.885565147
129	H	0.417049593	0.581967097	0.220083134
130	H	0.501991707	0.312436935	0.776674308
131	H	0.042359807	0.097223772	0.300970965
132	H	0.907837966	0.914100830	0.719496730
133	H	0.321725520	0.566341235	0.359201275
134	H	0.586237449	0.320370690	0.633174889
135	H	0.133744552	0.083578703	0.160239949

136	H	0.816044259	0.921203345	0.860384225
137	H	0.775006703	0.630040953	0.366042863
138	H	0.180757531	0.373281513	0.650826989
139	H	0.682159306	0.127499643	0.158107663
140	H	0.271347568	0.863636984	0.862849435
141	H	0.949524892	0.483264051	0.194701162
142	H	0.018912384	0.512389430	0.831100978
143	H	0.512409902	0.980127889	0.331725766
144	H	0.441711427	0.029006531	0.698062841
145	H	0.105529134	0.550739839	0.311739390
146	H	0.855464755	0.451489279	0.716186459
147	H	0.353581310	0.047108968	0.216101966
148	H	0.599384684	0.958349035	0.812977095
149	H	0.276884685	0.676234529	0.507410161
150	H	0.676429303	0.344100060	0.509548194
151	H	0.182636945	0.161461309	0.016018360
152	H	0.769705602	0.829992236	0.005460014
153	H	0.068126226	0.418298689	0.439323240
154	H	0.895969584	0.585739722	0.593449057
155	H	0.396821135	0.912231859	0.090916570
156	H	0.554413849	0.083133348	0.941789069
157	H	0.290323647	0.350602669	0.474325922
158	H	0.675392981	0.664874805	0.561497183
159	H	0.178904722	0.836718839	0.052611395
160	H	0.773735407	0.156574073	0.978321185
161	H	0.064894990	0.888404920	0.540743758
162	H	0.876883398	0.117210988	0.485676768
163	H	0.385138566	0.382156583	0.982770441
164	H	0.569432721	0.608617639	0.038964734
165	H	0.099124181	0.582485157	0.628770340
166	H	0.868312942	0.420859651	0.392359899
167	H	0.359372049	0.073699738	0.899240083
168	H	0.587003675	0.914655696	0.127953391
169	H	0.184038685	0.722640278	0.739868251
170	H	0.787218126	0.280438664	0.279996903
171	H	0.268462697	0.209098473	0.786558450
172	H	0.674654576	0.777050968	0.239805829
173	H	0.464888182	0.969150261	0.550472216
174	H	0.343851075	0.890278670	0.567320954
175	H	0.465526463	0.831236965	0.531820962
176	H	0.377611801	0.916525631	0.470836045

S3.7. IM

Energy (eV): -1148.57

Simulation cell vectos (Å):

a =	11.7950000762999991	0.0000000000000000	0.0000000000000000
b =	-0.0156551823000000	12.8139905664999993	0.0000000000000000
c =	-1.4527354561000001	0.0073720601000000	17.4094911285999991

Fractional coordinates:

No.	Element	X	Y	Z
1	Zn	0.668722439	0.529984027	0.211591647
2	Zn	0.287895788	0.453913798	0.812384862
3	Zn	0.783452969	0.045103981	0.318921061
4	Zn	0.171126681	0.967903393	0.710119994
5	Cu	0.015731828	0.676793925	0.454434095
6	Cu	0.933981316	0.341494234	0.570973041
7	Cu	0.449524196	0.160983135	0.064175486
8	Cu	0.511474757	0.828467993	0.959336248
9	Cu	0.481701466	0.529549421	0.520338167
10	Cu	0.978709955	0.997879955	0.015955052
11	N	0.651679395	0.414308448	0.133896943
12	N	0.318097870	0.572840047	0.883806028
13	N	0.806828716	0.925502165	0.390943334
14	N	0.142331662	0.088822564	0.638752658
15	N	0.559545843	0.278314001	0.077141489
16	N	0.405496334	0.709888662	0.941889396
17	N	0.902320546	0.789312124	0.443698161
18	N	0.043472265	0.222689926	0.584590549
19	N	0.558018313	0.493617410	0.287242178
20	N	0.393928145	0.439730293	0.728280701
21	N	0.899432006	0.035736763	0.241672900
22	N	0.056915044	0.974220904	0.788566519
23	N	0.490815505	0.443833701	0.398997953
24	N	0.459062399	0.453710777	0.612754717
25	N	0.972870028	0.021373722	0.128018635
26	N	0.984453741	0.980698856	0.902980308
27	N	0.821798909	0.551682896	0.268328863
28	N	0.132238811	0.450324537	0.758633430
29	N	0.632882349	0.053682403	0.259531943
30	N	0.323243203	0.949604284	0.768076024
31	N	0.952144479	0.610669074	0.358546257
32	N	-0.003032052	0.399967951	0.669061361
33	N	0.506104645	0.102574400	0.164102687
34	N	0.451684138	0.891485000	0.859927273
35	N	0.148984505	0.582737975	0.460028793
36	N	0.812689667	0.450787520	0.561553079
37	N	0.323380454	0.058541427	0.055492079
38	N	0.636016525	0.931047211	0.970812291
39	N	0.323079699	0.531695059	0.498956196
40	N	0.640499749	0.519560034	0.540309465

41	N	0.145814311	0.999766088	0.030852329
42	N	0.811403719	0.992184483	0.001344797
43	N	0.069806888	0.727667200	0.557539150
44	N	0.881907879	0.288498586	0.469028413
45	N	0.394251311	0.213668264	0.961571190
46	N	0.562564769	0.773621718	0.062843188
47	N	0.136727237	0.836753662	0.650339080
48	N	0.819839458	0.177714641	0.376133332
49	N	0.317400925	0.322959874	0.872172734
50	N	0.628322531	0.662954284	0.155189554
51	O	0.495744512	0.658237707	0.474014845
52	C	0.577953042	0.335299387	0.141762217
53	C	0.393187923	0.651152169	0.877854711
54	C	0.884873968	0.850989305	0.381447550
55	C	0.062715413	0.162421100	0.647539261
56	C	0.682729652	0.407012438	0.059464754
57	C	0.279718180	0.582593303	0.956198168
58	C	0.771790658	0.910113905	0.463690023
59	C	0.176472714	0.103479250	0.565639157
60	C	0.625655789	0.323539592	0.024464965
61	C	0.334004550	0.666798045	0.991990996
62	C	0.831168596	0.826479137	0.496296930
63	C	0.115289315	0.185653536	0.532232282
64	C	0.582719499	0.469322754	0.362242935
65	C	0.390966341	0.495443250	0.663011272
66	C	0.882525798	0.002682598	0.168498021
67	C	0.075775155	-0.000859242	0.863359438
68	C	0.441344657	0.482097148	0.274808622
69	C	0.467880695	0.357853602	0.718987251
70	C	0.007501713	0.078289884	0.248712090
71	C	0.946482030	0.937322328	0.779481899
72	C	0.400857241	0.451459838	0.343272713
73	C	0.508660718	0.366678142	0.647631179
74	C	0.053002011	0.068930528	0.179011715
75	C	0.901665702	0.941815854	0.849673036
76	C	0.840584052	0.605893864	0.334220557
77	C	0.109452935	0.404795532	0.689689515
78	C	0.616792461	0.099392593	0.190096784
79	C	0.340544724	0.896745510	0.834820092
80	C	0.927885881	0.520713096	0.248947604
81	C	0.027823256	0.475330329	0.784098044
82	C	0.525875108	0.026593087	0.279536742
83	C	0.430001978	0.978874017	0.748920333
84	C	0.008180464	0.556752444	0.304515041
85	C	0.944356530	0.444455356	0.728832191
86	C	0.447659422	0.056542776	0.220668636

87	C	0.509074000	0.943290865	0.805437304
88	C	0.257139528	0.613469148	0.476973684
89	C	0.703715972	0.432622338	0.535797798
90	C	0.214710075	0.083516978	0.032838273
91	C	0.744298946	0.907209428	0.995665677
92	C	0.146672178	0.475952973	0.471455491
93	C	0.818238513	0.554681522	0.583421173
94	C	0.323788142	0.952337077	0.068555720
95	C	0.633999543	0.037776621	0.960539044
96	C	0.254821396	0.443819888	0.496265034
97	C	0.711318738	0.597493212	0.570113628
98	C	0.214038522	0.916066285	0.053086764
99	C	0.742341944	0.075480715	0.979590045
100	C	0.087195147	0.827981862	0.578394972
101	C	0.856503564	0.188471071	0.450725322
102	C	0.370807552	0.313800385	0.943031105
103	C	0.582657994	0.673036515	0.082326083
104	C	0.110969871	0.668541645	0.619974854
105	C	0.860702132	0.344906006	0.401914830
106	C	0.353755836	0.155318094	0.898601774
107	C	0.597645499	0.831317841	0.127464692
108	C	0.151440408	0.735877015	0.677358900
109	C	0.822842330	0.276471176	0.344620696
110	C	0.306737866	0.222629975	0.843375154
111	C	0.637624329	0.763121830	0.184325097
112	C	0.438049682	0.914755175	0.497600052
113	H	0.537668177	0.320131469	0.194273691
114	H	0.438314729	0.665375632	0.827178083
115	H	0.928661364	0.842341680	0.329585672
116	H	0.019366753	0.171523854	0.699556152
117	H	0.742392288	0.461316531	0.037030457
118	H	0.217465035	0.529215460	0.976679632
119	H	0.706521698	0.958137143	0.486200255
120	H	0.240605274	0.054323460	0.542847263
121	H	0.626184178	0.294124871	0.966333317
122	H	0.328311438	0.698155433	0.049130141
123	H	0.828841035	0.791372804	0.552516317
124	H	0.116535896	0.219300080	0.475331727
125	H	0.669002175	0.469754691	0.389024787
126	H	0.338787760	0.564255613	0.651297783
127	H	0.805018104	0.965028254	0.144980758
128	H	0.155313569	0.031054933	0.888619128
129	H	0.396730412	0.497010201	0.218986513
130	H	0.484751326	0.299050561	0.763132320
131	H	0.042939292	0.112900718	0.302131369
132	H	0.908967697	0.909736082	0.724340901

133	H	0.313967391	0.435685746	0.356042680
134	H	0.568402415	0.318405540	0.619922839
135	H	0.135370033	0.092944873	0.162112330
136	H	0.818033271	0.919837863	0.865411615
137	H	0.774051993	0.641436021	0.364691023
138	H	0.174174802	0.375616203	0.654644249
139	H	0.684856564	0.129973019	0.158479408
140	H	0.272874635	0.863021916	0.865323042
141	H	0.938242732	0.474867799	0.197807955
142	H	0.020635992	0.513441852	0.838904996
143	H	0.513536564	0.987996029	0.333530689
144	H	0.441713152	0.023239220	0.697250590
145	H	0.099829211	0.547850885	0.309994250
146	H	0.852639618	0.451754030	0.727183973
147	H	0.356009338	0.047454403	0.214594997
148	H	0.600747510	0.952316818	0.811342801
149	H	0.288910130	0.692548743	0.473864919
150	H	0.671507362	0.359468250	0.511618790
151	H	0.186719003	0.161862582	0.017139446
152	H	0.773103647	0.828742734	0.010204837
153	H	0.069427842	0.430738131	0.459450433
154	H	0.896908504	0.590177966	0.607144855
155	H	0.400184849	0.911037844	0.089642026
156	H	0.557555862	0.078617883	0.938935787
157	H	0.288351038	0.367072096	0.510932766
158	H	0.679744335	0.675902809	0.577143678
159	H	0.180055645	0.837683730	0.056404169
160	H	0.774441311	0.154801096	0.979461548
161	H	0.063668213	0.894083090	0.541629796
162	H	0.866167018	0.123972504	0.491013931
163	H	0.393340823	0.379519552	0.980404920
164	H	0.563737028	0.607608840	0.043953022
165	H	0.108713173	0.583930966	0.619028781
166	H	0.873586766	0.428574129	0.399923847
167	H	0.360912625	0.071062591	0.897885331
168	H	0.591987983	0.915738503	0.128312294
169	H	0.188080896	0.719429920	0.735158725
170	H	0.798044748	0.290985307	0.284369043
171	H	0.267442981	0.206720654	0.786168836
172	H	0.671336872	0.778829417	0.242886754
173	H	0.461130874	0.953474558	0.552105461
174	H	0.459240241	0.832759805	0.490036671
175	H	0.526086272	0.643708511	0.424790379
176	H	0.393577837	0.958733565	0.451021266

S3.8. TS

Energy (eV): -1148.41

Simulation cell vectos (Å):

a =	11.7950000762999991	0.0000000000000000	0.0000000000000000
b =	-0.0156551823000000	12.8139905664999993	0.0000000000000000
c =	-1.4527354561000001	0.0073720601000000	17.4094911285999991

Fractional coordinates:

No.	Element	X	Y	Z
1	Zn	0.670256205	0.529968835	0.210559255
2	Zn	0.285415500	0.456847518	0.814254569
3	Zn	0.783717805	0.041022292	0.318002988
4	Zn	0.171984822	0.965141324	0.709656486
5	Cu	0.014036855	0.671579634	0.455927999
6	Cu	0.938192357	0.337913852	0.569300025
7	Cu	0.449022771	0.160948096	0.064038940
8	Cu	0.510346192	0.829694233	0.960445817
9	Cu	0.480364470	0.518889343	0.515811914
10	Cu	0.978599649	0.997231584	0.014692291
11	N	0.651230974	0.414186796	0.133706742
12	N	0.313751003	0.575164686	0.886581856
13	N	0.807530369	0.922003205	0.390513073
14	N	0.144786203	0.085212097	0.637665313
15	N	0.559060094	0.278112040	0.077232324
16	N	0.403247040	0.711604904	0.944046814
17	N	0.901974209	0.785671294	0.444053878
18	N	0.047573074	0.219591864	0.582979534
19	N	0.558145539	0.499514126	0.286798455
20	N	0.395044822	0.448981259	0.732727472
21	N	0.899468748	0.032664431	0.240654183
22	N	0.057242321	0.971516073	0.787697161
23	N	0.487638194	0.464750393	0.399460328
24	N	0.462224893	0.460209774	0.617307168
25	N	0.972525108	0.020096343	0.126786195
26	N	0.984647333	0.978673540	0.902013492
27	N	0.822673246	0.549772792	0.267673576
28	N	0.131362016	0.449613850	0.758809426
29	N	0.632887959	0.051388695	0.258842795
30	N	0.323563837	0.948364216	0.768219026
31	N	0.952375371	0.607442446	0.358728338
32	N	0.999106574	0.396760653	0.668073670
33	N	0.506088845	0.102100957	0.163931692

34	N	0.451376576	0.891768358	0.860897510
35	N	0.143883840	0.574124595	0.463349874
36	N	0.815927515	0.444975464	0.559506408
37	N	0.323159374	0.058407293	0.055000990
38	N	0.635088336	0.932377392	0.971535363
39	N	0.318677044	0.519684723	0.498647158
40	N	0.641861140	0.510603800	0.536126452
41	N	0.145747430	0.999471341	0.029856445
42	N	0.811295390	0.992555963	0.000004209
43	N	0.068516581	0.723996861	0.558570948
44	N	0.885318861	0.284325330	0.467148618
45	N	0.393406859	0.214822453	0.961860777
46	N	0.562613822	0.774464824	0.063429930
47	N	0.137480389	0.833788555	0.650276895
48	N	0.819448644	0.173429899	0.375411065
49	N	0.316492857	0.325071911	0.873128099
50	N	0.630158231	0.663152164	0.154708507
51	O	0.488803815	0.667939924	0.493400275
52	C	0.577608735	0.335163381	0.141788983
53	C	0.389095451	0.653099391	0.879984406
54	C	0.884744719	0.846612033	0.381387369
55	C	0.066807325	0.160230084	0.646362742
56	C	0.681997992	0.406847648	0.059213806
57	C	0.277196218	0.584845715	0.959450896
58	C	0.772994218	0.908090783	0.463546341
59	C	0.177752751	0.097853560	0.564101153
60	C	0.624873684	0.323301485	0.024392816
61	C	0.332777475	0.668660526	0.994881978
62	C	0.831625587	0.824319132	0.496587989
63	C	0.117521019	0.180322543	0.530367854
64	C	0.581578839	0.480466680	0.362349003
65	C	0.388051138	0.496903872	0.664589674
66	C	0.882708005	0.999920954	0.167394192
67	C	0.075591057	0.997923661	0.862223345
68	C	0.441367084	0.494896168	0.274171422
69	C	0.479186021	0.377205520	0.729012392
70	C	0.006819479	0.076693476	0.247574175
71	C	0.947617304	0.932699528	0.778992914
72	C	0.398831967	0.473284772	0.343120851
73	C	0.521491556	0.384318497	0.658088032
74	C	0.052103528	0.068411701	0.177736499
75	C	0.902683235	0.937630896	0.849127964
76	C	0.841131222	0.603683369	0.333722430
77	C	0.111054743	0.402712536	0.690152324
78	C	0.616860653	0.097824749	0.189644162
79	C	0.340377288	0.896768893	0.835481736

80	C	0.928708959	0.517904190	0.248897001
81	C	0.025851401	0.474344232	0.782495678
82	C	0.525736779	0.025096260	0.278979187
83	C	0.430480332	0.977141797	0.749075457
84	C	0.008594076	0.553157559	0.304999560
85	C	0.944253757	0.441949011	0.726523567
86	C	0.447523090	0.056154632	0.220454844
87	C	0.509198927	0.942496833	0.806121559
88	C	0.252541589	0.602594578	0.481624309
89	C	0.707277775	0.424519052	0.534047027
90	C	0.214659834	0.083183448	0.031649909
91	C	0.743517052	0.908041841	0.995545602
92	C	0.140817951	0.467049031	0.469344400
93	C	0.819286116	0.549471693	0.579227576
94	C	0.323381358	0.952352118	0.068707011
95	C	0.633708006	0.038968163	0.960452577
96	C	0.249053948	0.432947821	0.492126364
97	C	0.711401728	0.589898998	0.565002674
98	C	0.213737915	0.915995264	0.052931207
99	C	0.742570602	0.076094258	0.978274433
100	C	0.088099208	0.824360545	0.578321013
101	C	0.860342377	0.184163752	0.449117107
102	C	0.368905376	0.315048254	0.944182829
103	C	0.583588302	0.673812508	0.082126563
104	C	0.107849486	0.665605744	0.621784389
105	C	0.859173209	0.340887120	0.400796134
106	C	0.354584620	0.157347512	0.898079676
107	C	0.597938344	0.831584898	0.128237898
108	C	0.149645275	0.733354087	0.678466728
109	C	0.819027137	0.272433510	0.344194246
110	C	0.307608219	0.225291717	0.843266414
111	C	0.639016405	0.762971708	0.184497192
112	C	0.425346813	0.902795824	0.497024228
113	H	0.537623434	0.319939056	0.194413408
114	H	0.433182003	0.666981548	0.828819535
115	H	0.928072956	0.836781489	0.329450393
116	H	0.024483903	0.170980228	0.698603955
117	H	0.741492529	0.461176880	0.036629657
118	H	0.215156321	0.531716612	0.980485551
119	H	0.709276279	0.957734582	0.486158211
120	H	0.240582653	0.047342868	0.541284553
121	H	0.625142161	0.293791174	0.966274968
122	H	0.328607305	0.699823694	0.052206546
123	H	0.829229619	0.790068384	0.553099235
124	H	0.118271953	0.212835165	0.473113611
125	H	0.667168571	0.477487332	0.389790112

126	H	0.328390773	0.557223875	0.648769164
127	H	0.805663091	0.961448064	0.143941402
128	H	0.154495427	0.031441725	0.887150885
129	H	0.397965225	0.507794215	0.217750546
130	H	0.501358472	0.325815903	0.776384038
131	H	0.041878070	0.111510084	0.301011143
132	H	0.910754345	0.903573092	0.724156929
133	H	0.311514294	0.463799269	0.356073618
134	H	0.588094910	0.341830990	0.633992614
135	H	0.133981009	0.093600471	0.160701570
136	H	0.819532796	0.914587794	0.865133568
137	H	0.774567106	0.639804343	0.363791613
138	H	0.177158077	0.373589418	0.656261740
139	H	0.685064285	0.127963006	0.157942182
140	H	0.272499806	0.863682432	0.866100894
141	H	0.939284873	0.471984443	0.197831434
142	H	0.016664135	0.513409714	0.836657559
143	H	0.513199505	0.986185630	0.332815834
144	H	0.442540605	0.020653385	0.697086212
145	H	0.100051796	0.543146881	0.311084976
146	H	0.852443190	0.448803316	0.723517907
147	H	0.355788914	0.047792836	0.214542220
148	H	0.600870479	0.951469575	0.812191497
149	H	0.284273367	0.681627762	0.482802698
150	H	0.676929638	0.349778229	0.511873551
151	H	0.186872966	0.161355937	0.015323568
152	H	0.771967307	0.829549536	0.010355389
153	H	0.063367434	0.423194226	0.455185764
154	H	0.896977484	0.586876147	0.602614004
155	H	0.399606487	0.911217858	0.090331445
156	H	0.557299679	0.080036859	0.939065590
157	H	0.281620577	0.355146523	0.503113986
158	H	0.678340326	0.667978332	0.570965240
159	H	0.179708241	0.837659836	0.056465250
160	H	0.775315254	0.155118849	0.977252754
161	H	0.066025512	0.890065093	0.540856171
162	H	0.873172650	0.119550899	0.488963123
163	H	0.390062378	0.380242919	0.982324548
164	H	0.564562150	0.608765795	0.043415500
165	H	0.103583618	0.581125559	0.621780220
166	H	0.870504862	0.424720832	0.398810026
167	H	0.362731163	0.073208402	0.896541511
168	H	0.591734128	0.915930469	0.129575594
169	H	0.185706054	0.717482561	0.736482638
170	H	0.790678334	0.286983866	0.284561765
171	H	0.269623049	0.210132812	0.785630640

172	H	0.673308345	0.778126442	0.243014418
173	H	0.484633696	0.963908028	0.517214195
174	H	0.429367460	0.825775854	0.523508609
175	H	0.517652265	0.674790865	0.442904736
176	H	0.368341000	0.916809982	0.445799927

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