Supporting Information

p-Block doped semi-metallic xenes as highly selective and efficient transition-metal free single atom catalysts for electrochemical CO reduction

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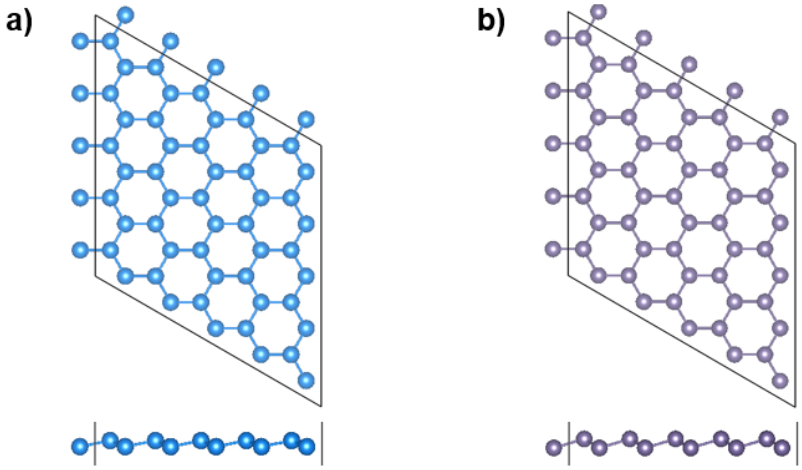

Figure S1 Schematics for (a) pristine Silicene (Si) and (b) Germanene (Ge) from top and side views. Color code: Si – light blue, Ge – violet.

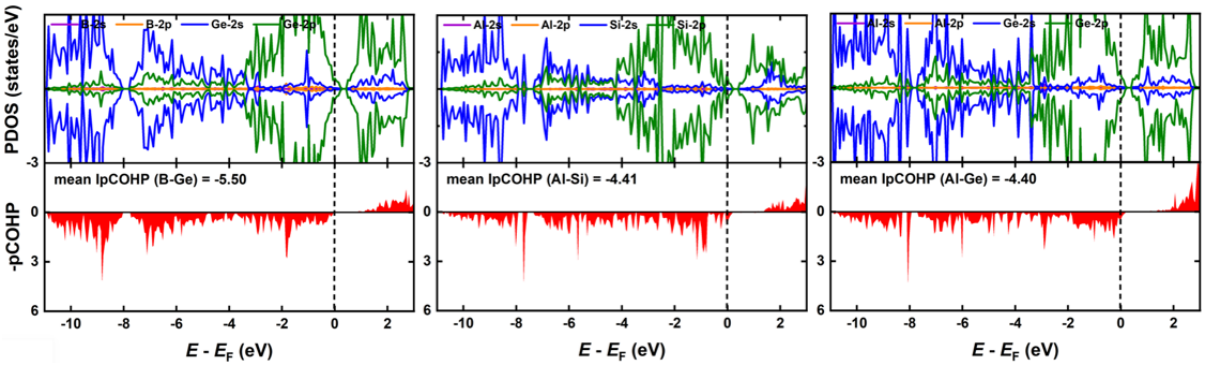

Fig. S2 The PDOS projected on the *s* and *p* orbitals of dopants and host substrates in B@Ge, Al@Si and Al@Ge; The pCOHP of the B-Ge, Al-Si and Al-Ge bonds. The pCOHP of the spin-down component is masked by that of the spin-up. The Fermi energy is set at zero.

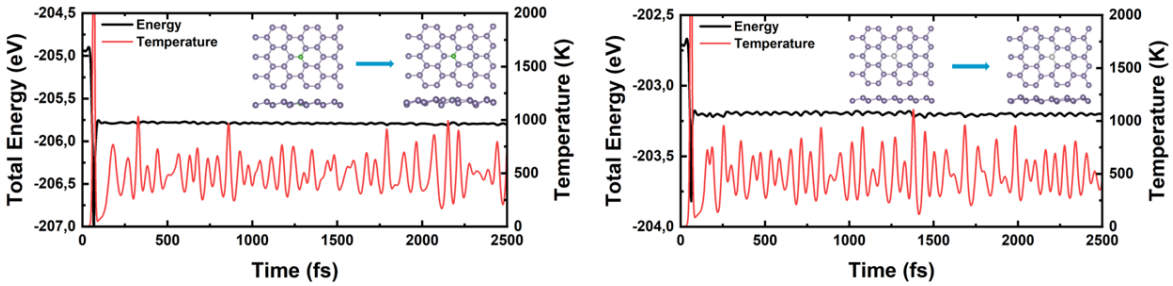

Fig. S3 *AIMD* simulations of B@Ge and Al@Ge at 500 K with their initial and final structures. Color code: B - green, Al – silver, Ge – violet.

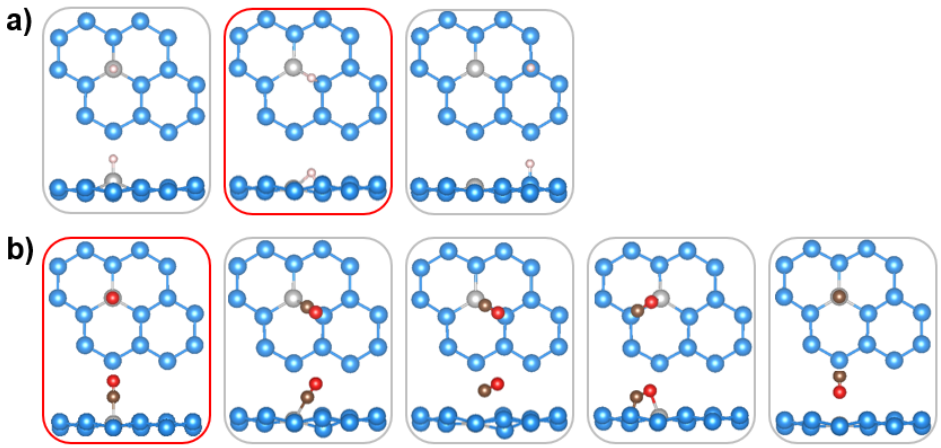

Figure S4 Possible optimized configurations of (a) H* adsorption for HER and (b) CO* adsorption for CORR on catalytic system. Red box line indicates the lowest-energy geometry. Take Al@Si structure as an example. Color code: Al – silver, Si – light blue, C – brown, O – red, H – light pink.

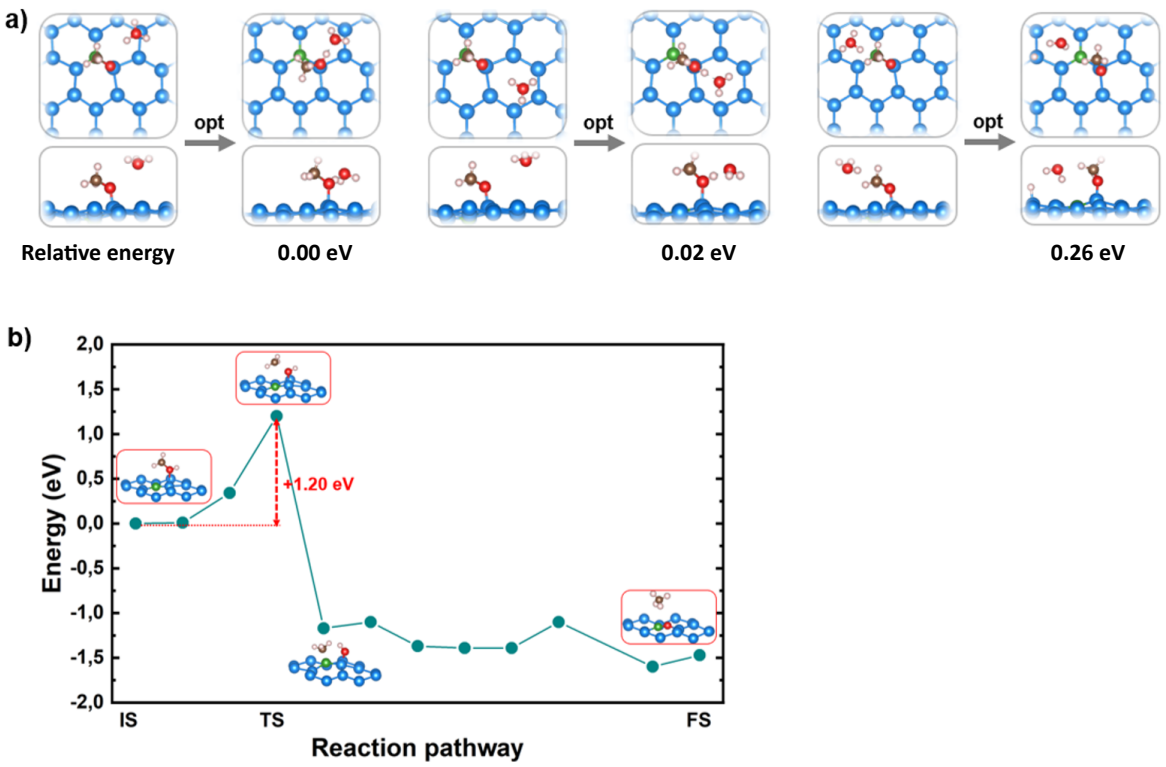

Figure S5 (a) Top and side views of CH_3O*-adsorbed B@Si configurations in the presence of H_3O^+ before and after structure optimization. Starting geometries with H_3O^+ placed in the vicinity of CH_3O with access to both CH_3 and O result in binding to O and the spontaneous transfer of the proton to form CH_3OH*. Placing the H_3O^+ with access only to CH_3 results in the H_3O^+ binding to a nearby Si and the proton being transferred. The CH_3OH* structures are lower in energy than the (H(Si)*/CH_3O*) structure by 0.25 eV. **(b)** The reaction path energy diagram for the elementary chemical step $CH_3OH^* \rightarrow O^* + CH_4$ as obtained by nudge elastic band (NEB) calculations. Red insets show the atomic structures of initial state (IS), transition state (TS) and final state (FS). Color code: B – green, Si – light blue, C – brown, O – red, H – light pink.

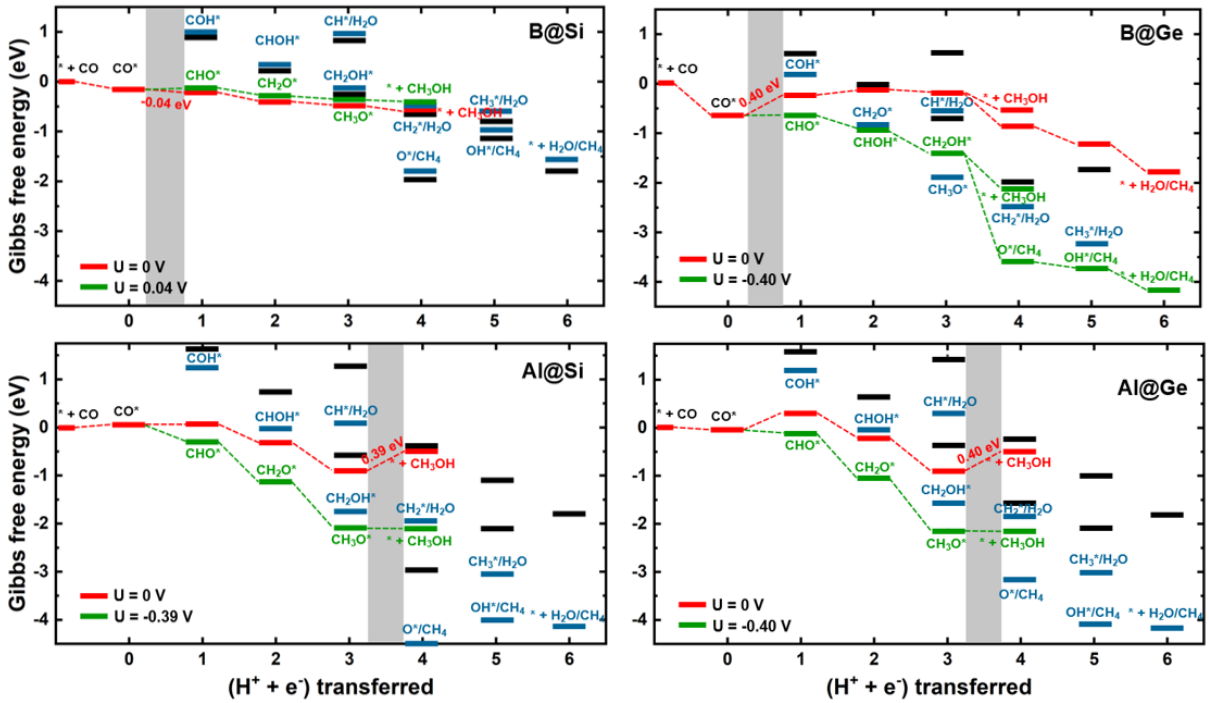

Fig. S6 Free-energy profiles for CO reduction with applied potentials on four model systems. The red and green lines (bars) represent the most favorable pathways, while the black and dark blue bars illustrate possible pathways without and with applied limiting potentials, respectively. Note that for B@Si the limiting potential is close to 0 V and thus the application of the limiting potential ($U = U_L$) has little effect compared $U = 0$ V.

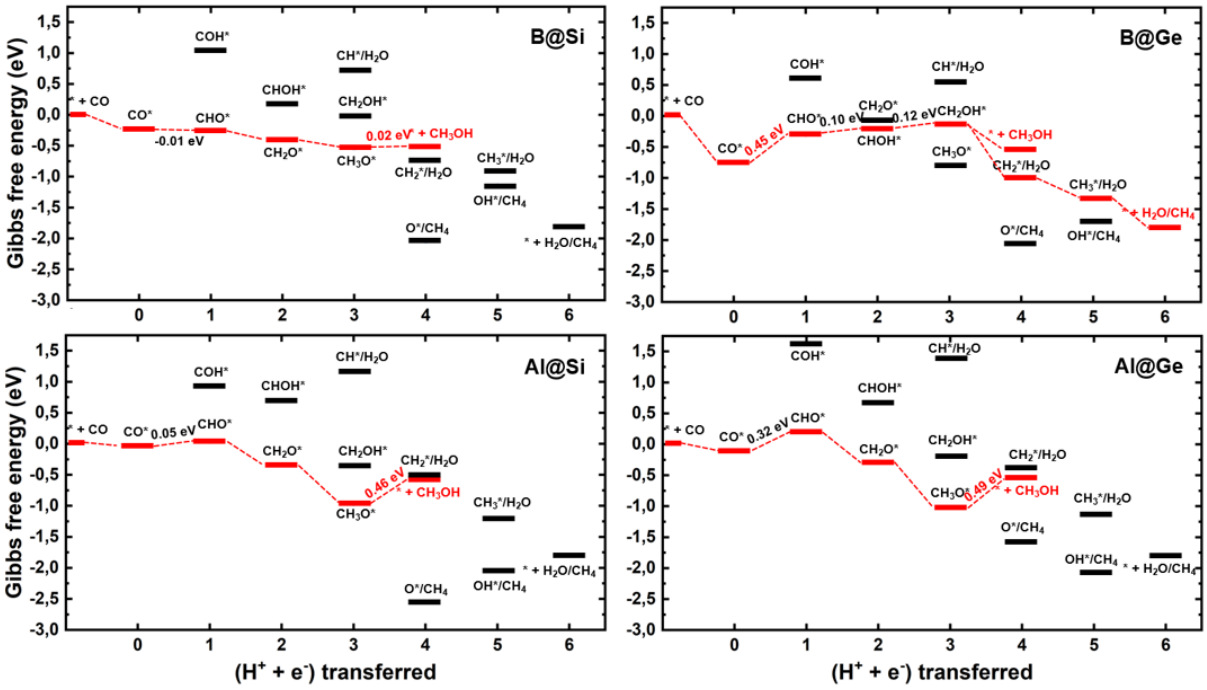

Fig. S7 Free-energy profiles for CO reduction in vacuum on four model systems. The red line and the number display the most favorable overall pathway and the lowest limiting potential value, respectively.

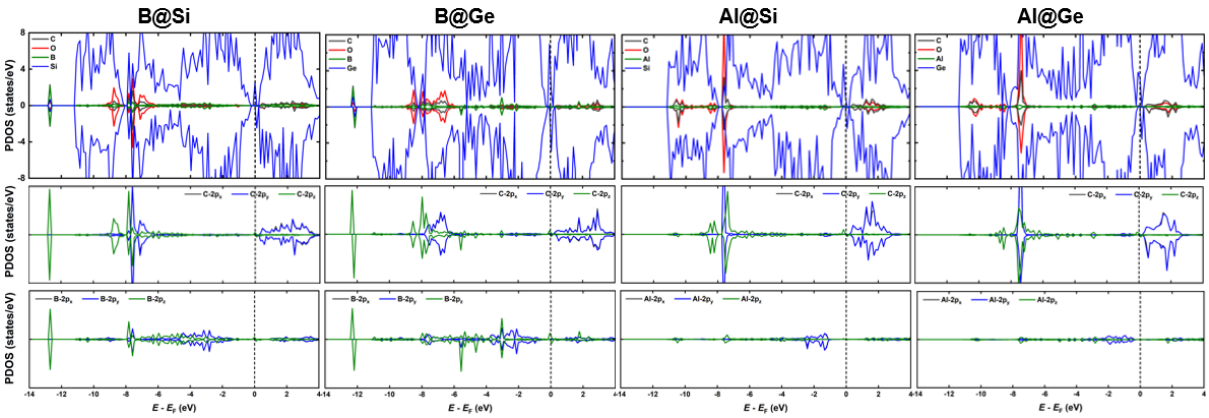

Figure S8 Partial density of states (PDOS) of C, O, B/Al and Si/Ge elements (topmost), C(p_x, p_y, p_z) orbitals (middle), and B(p_x, p_y, p_z) orbitals (bottom panels) of CO adsorption on four systems. Note p_x orbital is masked by p_y orbital.

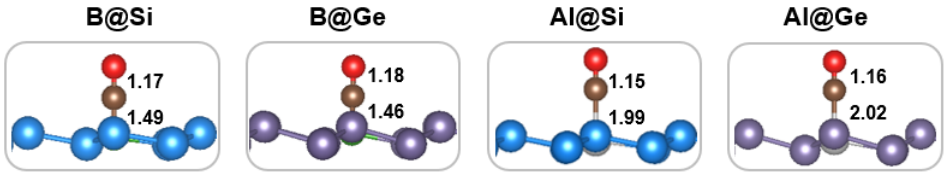

Figure S9 Optimized configurations of CO* adsorption on four systems and their two corresponding bond lengths of C-B/Al and C-O. Unit: Å

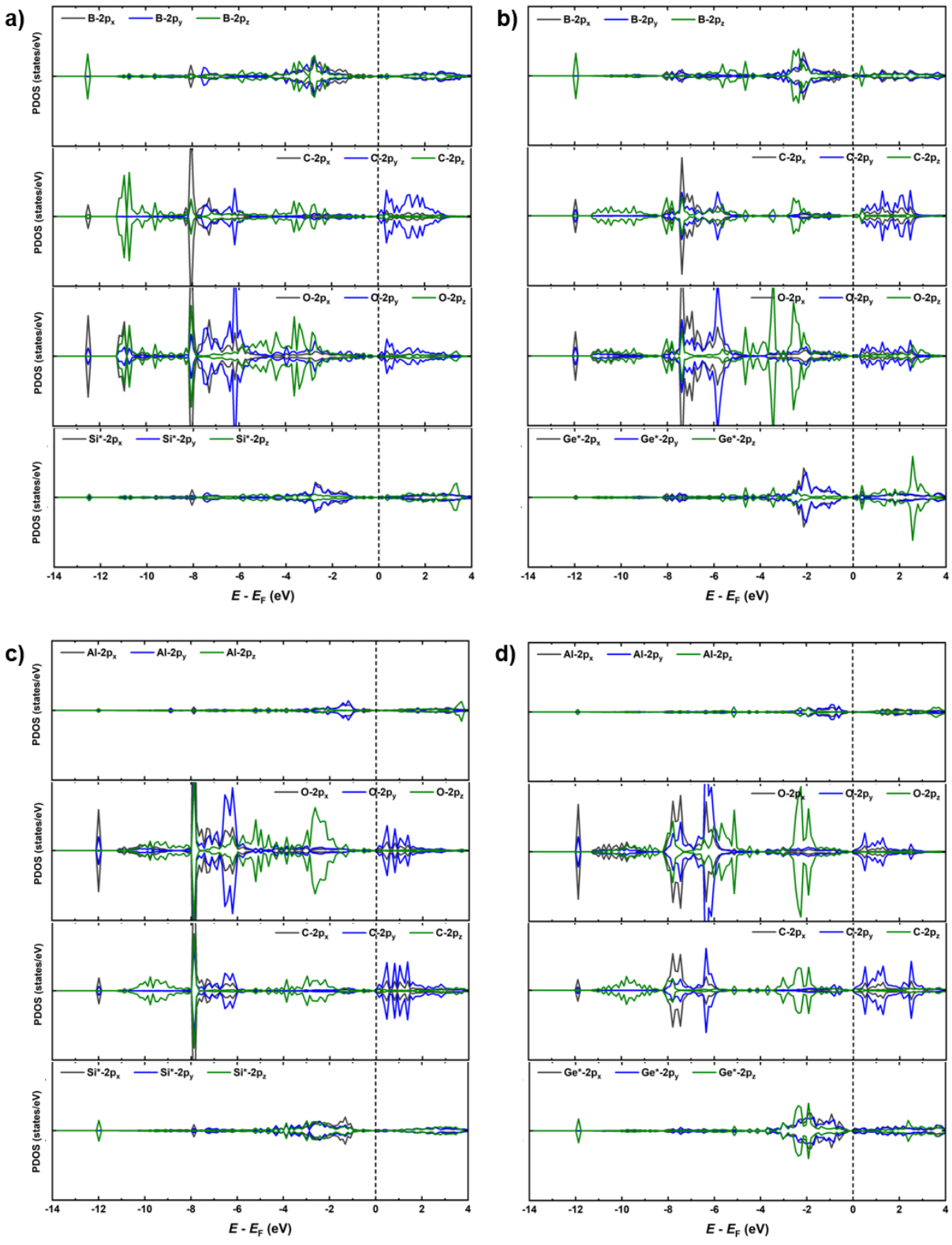

Figure S10 Partial density of states (PDOS) of B/Al (p_x, p_y, p_z), O(p_x, p_y, p_z), C(p_x, p_y, p_z) and host atom (Si*/Ge*)(p_x, p_y, p_z) orbitals of CHO* adsorption on a) B@Si, b) B@Ge, c) Al@Si and d) Al@Ge.

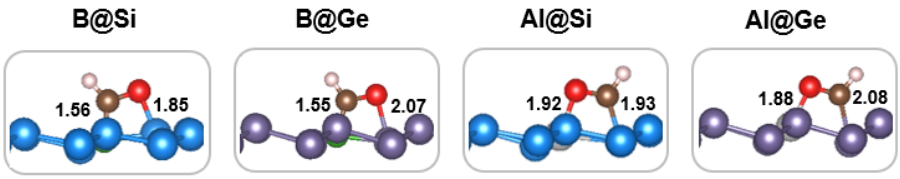

Figure S11 Optimized configurations of CHO* adsorption on four systems and their two corresponding bond lengths of dual active sites and C/O (CHO*). Unit: Å

System	B@Si	B@Ge	Al@Si	Al@Ge
E_{ads}[CO*]	-0.76	-1.27	-0.48	-0.52
E_{ads}[CHO*]	-1.13	-1.19	-0.82	-0.62
U_L	-0.04	0.40	0.02	0.29

Table S1 Adsorption energies (eV) of two CO* and CHO* intermediates, E_{ads}[CO*] and E_{ads}[CHO*]; and limiting potential (U_L)(V) for CORR on each model systems.

Optimized lowest-energy intermediate geometries in Figure 4

CO ads BSi

1.0

19.3415393829 0.0000000000 0.0000000000

-9.6707696915 16.7502644539 0.0000000000

0.0000000000 0.0000000000 20.0017776489

Si B C O

49 1 1 1

Cartesian

0.007791379 2.254163742 3.593504429

-1.924107075 5.589223862 3.592967749

-3.846404314 8.929826736 3.593501091

-5.802462578 12.279019356 3.599550962

-7.740522385	15.635837555	3.599550247
3.868306637	2.240489483	3.591114521
1.965131879	5.658411980	3.568762541
0.080432393	8.922808647	3.568758726
-1.927987814	12.279969215	3.591114044
-3.864403009	15.635837555	3.599551439
7.728824139	2.254163265	3.593502045
5.771482468	5.658411980	3.568759441
1.983607888	12.219205856	3.568759441
0.014111436	15.616436005	3.593501329
11.602069855	2.231722116	3.597829103
9.660722733	5.589223385	3.592967749
7.656183720	8.922809601	3.568758965
5.753007889	12.219206810	3.568763018
3.868307352	15.621979713	3.592967749
15.476084709	2.231722355	3.597828627
13.539077759	5.586717606	3.597828627
11.583019257	8.929826736	3.593502045
9.664602280	12.279970169	3.591114521
7.722503185	15.616436958	3.593504429
1.930417895	1.121956348	3.151313066
0.024838088	4.503617287	3.166509867
-1.889797091	7.819862366	3.166510344
-3.865612030	11.160975456	3.151313543
-5.802463055	14.516898155	3.147726297
5.806196213	1.121955991	3.151315451
3.868306875	4.467101097	3.177396774
2.069460154	7.894909859	3.137248993
0.000313949	11.166663170	3.177396774
-1.927723289	14.517498016	3.151313543
9.665306091	1.113530874	3.156387329
7.711777687	4.503617287	3.166510344
5.667153835	7.894911289	3.137249708
3.868308306	11.010605812	3.137248993
1.953672647	14.476947784	3.166510344
13.539076805	1.112864375	3.153178692

11.601614952 4.468648434 3.153177261
9.626413345 7.819862366 3.166510582
7.736300945 11.166664124 3.177396536
5.782943249 14.476947784 3.166509867
17.412849426 1.113530874 3.156388521
15.476538658 4.468648911 3.153179169
13.539076805 7.823100090 3.156387568
11.602225304 11.160975456 3.151315451
9.664336205 14.517498016 3.151313066
3.868305922 8.933476448 3.446789265
3.868313074 8.933472633 4.908610344
3.868319988 8.933467865 6.081818104

CHO ads BSi

1.0

19.3415393829 0.0000000000 0.0000000000
-9.6707696915 16.7502644539 0.0000000000
0.0000000000 0.0000000000 20.0017776489

Si B C O H

49 1 1 1 1

Cartesian

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-1.933440566 5.578364849 3.593802691
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-5.800652981 12.280582428 3.594871283
-7.737428188 15.642781258 3.592027664
3.872960091 2.250726700 3.572744608
1.954607964 5.689144135 3.553002834
0.059120916 8.902019501 3.527076721
-1.935786366 12.284557343 3.590675592
-3.862925529 15.636887550 3.594616413
7.727843761 2.267633438 3.581505060
5.784232616 5.673136234 3.593365192
1.982079506 12.234135628 3.546670675
0.005304948 15.629499435 3.593930483

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7.761083603	8.949632645	3.509855747
5.715501785	12.189104080	3.567131042
3.873632669	15.623918533	3.590152264
15.474409103	2.230346680	3.600108862
13.539640427	5.580942154	3.596514940
11.602116585	8.933105469	3.584909439
9.675011635	12.295095444	3.581614494
7.715084076	15.610846519	3.594630957
1.934376597	1.128392935	3.150691748
0.024539381	4.496353149	3.167527676
-1.917894602	7.814781189	3.172528744
-3.869399786	11.163932800	3.154134750
-5.801112652	14.518122673	3.159421921
5.807174683	1.124961376	3.155480146
3.888245583	4.509459496	3.192189217
2.041523933	7.907803535	3.003252268
-0.001547810	11.161176682	3.189010382
-1.930890203	14.520282745	3.152817249
9.664883614	1.123999953	3.156148672
7.701124668	4.524085522	3.172743082
5.612771034	8.020264626	3.568690300
3.828865290	10.977803230	3.047798872
1.944922686	14.491591454	3.166622400
13.540610313	1.114796996	3.154768944
11.599845886	4.466270924	3.151538849
9.673141479	7.802453518	3.106929779
7.732348919	11.173573494	3.166431904
5.780718327	14.453688622	3.168042183
17.405153275	1.107415438	3.158122540
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13.544512749	7.815922260	3.160229683
11.605401039	11.166624069	3.149494410

9.667970657 14.526999474 3.152529955

3.755389452 8.955270767 3.337961912

3.921498537 8.954319954 4.879082680

5.093536854 8.488005638 5.287804127

3.231821775 9.232267380 5.699052811

COH ads BSi

1.0

19.3415393829 0.0000000000 0.0000000000

-9.6707696915 16.7502644539 0.0000000000

0.0000000000 0.0000000000 20.0017776489

Si B C O H

49 1 1 1 1

Cartesian

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-3.827817202 8.931724548 3.575402260

-5.807874680 12.285222054 3.602392673

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3.867197990 2.251874685 3.585362196

1.984315753 5.648040771 3.699474335

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9.667832375 5.579864025 3.594609976

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15.475523949 2.235878944 3.599012613

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-5.804327488	14.517065048	3.146327019
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3.860937357	4.502149105	3.186516047
2.104340076	7.979753494	3.580366373
-0.006318716	11.174688339	3.170747280
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9.672625542	1.111173272	3.160009384
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13.542613983	1.110657573	3.156550646
11.609209061	4.463799000	3.153393269
9.678843498	7.814321995	3.171042681
7.731682777	11.169839859	3.188513994
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13.560750961	7.818060875	3.156315804
11.601915359	11.167051315	3.151274204
9.669804573	14.517430305	3.153412342
4.099864483	9.003389359	3.464257717
3.353196383	8.694608688	4.747143269
3.632062912	8.704706192	6.034699440
4.552425861	9.036132812	6.190460205

CH2O ads BSi

1.0

19.3415393829	0.0000000000	0.0000000000
-9.6707696915	16.7502644539	0.0000000000
0.0000000000	0.0000000000	20.0017776489

Si	B	C	O	H
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Cartesian

0.008798568	2.266129494	3.589584589
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-5.795132637	12.275967598	3.596287012
-7.741278648	15.636848450	3.586631298
3.871589661	2.240695715	3.556447983
1.970458627	5.720632553	3.404116631
0.095529288	8.893137932	3.390065908
-1.908018351	12.268750191	3.585927963
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7.740412712	2.231596947	3.574784756
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2.015951633	12.221214294	3.386448383
0.021164663	15.604553223	3.607378006
11.610931396	2.227216721	3.605553865
9.659132004	5.590353012	3.550010204
7.692737103	8.907759666	3.315290451
5.702924252	12.181871414	3.397944927
3.872752905	15.615143776	3.594453812
15.476442337	2.230788946	3.591931581
13.546449661	5.580677986	3.605283737
11.609868050	8.931883812	3.575223684
9.667264938	12.278282166	3.557090044
7.711546898	15.607378960	3.589189529
1.931145310	1.124810934	3.165230036
0.040593643	4.517613411	3.181699991
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-3.849882126 11.161496162 3.162411213

-5.798755646 14.514961243 3.157391787

5.805062771 1.116304755 3.144667625

3.880308867 4.484705925 3.156393766

2.117252350 7.949686527 2.928242445

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5.553757668 7.968209743 3.636075735

3.844393492 10.941919327 2.925297022

1.953905702 14.487064362 3.155457973

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11.599481583 4.469012737 3.167012691

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7.729874611 11.149456978 3.150773525

5.777923107 14.454336166 3.180374622

17.414712906 1.110895872 3.178060055

15.485399246 4.468880177 3.157248259

13.566560745 7.818305969 3.170642376

11.606982231 11.165413857 3.143971443

9.662807465 14.516285896 3.166213036

3.782769680 8.984347343 3.420938015

3.943186522 8.893773079 5.103617668

5.199824810 8.192385674 5.274770737

3.141211748 8.323148727 5.594739914

4.015225410 9.880850792 5.598987103

CHOH ads BSi

1.0

19.3415393829 0.0000000000 0.0000000000

-9.6707696915 16.7502644539 0.0000000000

0.0000000000 0.0000000000 20.0017776489

Si B C O H

49 1 1 1 2

Cartesian

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-3.827422857	8.926337242	3.603852987
-5.802697182	12.279568672	3.601206779
-7.742119312	15.622098923	3.596358776
3.878320932	2.234115601	3.616490126
1.974316597	5.673215866	3.513269663
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-1.911112428	12.269040108	3.593225002
-3.862143040	15.629524231	3.598824739
7.732845306	2.240288496	3.611599207
5.792274475	5.676668167	3.379349947
2.021989584	12.192174911	3.475014925
0.027845928	15.594482422	3.611023426
11.608435631	2.226788521	3.610069275
9.650373459	5.586741447	3.532882452
7.650212288	8.866907120	3.291193962
5.744234562	12.191020966	3.398375988
3.869257450	15.610862732	3.588927269
15.474743843	2.229625225	3.597599268
13.542933464	5.583904266	3.610147715
11.591749191	8.931449890	3.588202238
9.650971413	12.253403664	3.604639769
7.725697994	15.607589722	3.594339371
1.936817169	1.114805698	3.162279844
0.028564150	4.505094051	3.172129154
-1.871487379	7.815501213	3.150405407
-3.860886335	11.161567688	3.153805017
-5.800162315	14.512987137	3.148464441
5.809170246	1.113902450	3.136504412
3.875337839	4.459999084	3.173859358
2.162688971	7.921347618	3.165065289

0.018944858 11.150902748 3.164080143

-1.922820807 14.508294106 3.149233103

9.672784805 1.096657872 3.173533678

7.719938755 4.470513821 3.077010155

5.601768970 7.898579597 2.811735153

3.884773493 10.942026138 3.014370441

1.961700320 14.457896233 3.138025761

13.543089867 1.107389331 3.152631521

11.601716042 4.466966152 3.168626785

9.662355423 7.812139511 3.054454327

7.742579937 11.128996849 3.092154026

5.788044453 14.471755981 3.175014257

17.410259247 1.108576298 3.163754225

15.477564812 4.465785503 3.150612354

13.551636696 7.822067261 3.162308455

11.598583221 11.164022446 3.150001049

9.664116859 14.492865562 3.161997795

3.898033619 8.965374947 3.542146683

4.558459282 8.602476120 4.899749756

5.322984695 9.354913712 5.703569412

4.330567360 7.654107571 5.390426159

5.517677307 10.234467506 5.266283512

CH3O ads BSi

1.0

19.3415393829 0.0000000000 0.0000000000

-9.6707696915 16.7502644539 0.0000000000

0.0000000000 0.0000000000 20.0017776489

Si B C O H

49 1 1 1 3

Cartesian

0.014846630 2.264813900 3.601367235

-1.921823859 5.602067471 3.547333717

-3.843947411 8.930044174 3.598773479

-5.802032948	12.285372734	3.602643490
-7.736279488	15.632474899	3.589960098
3.862512112	2.227295637	3.540264368
1.975917697	5.709481716	3.211188555
0.107951313	8.917959213	3.208850384
-1.929358125	12.280001640	3.610597134
-3.869872570	15.631542206	3.603021860
7.722775936	2.254494905	3.551517963
5.743778706	5.696372032	3.324567318
2.001312494	12.196105957	3.212114573
0.015091628	15.613140106	3.599403381
11.596948624	2.235689402	3.591413021
9.649624825	5.594918251	3.522164822
7.607170105	8.926159859	3.329548836
5.713503838	12.183894157	3.215770483
3.857772589	15.612867355	3.548074007
15.473411560	2.232593060	3.578820229
13.532663345	5.588769436	3.591853380
11.578434944	8.934368134	3.552275896
9.672226906	12.290390968	3.540366888
7.716753006	15.604569435	3.601571083
1.922028780	1.110656381	3.154782772
0.032285687	4.511083126	3.143607616
-1.901937366	7.830909252	3.113509893
-3.866894722	11.166009903	3.170044422
-5.801827908	14.516200066	3.156687021
5.802330971	1.110995770	3.155416012
3.877715111	4.458459854	3.089207411
2.135338545	7.965998650	2.721198320
-0.016650077	11.176024437	3.059334517
-1.932908535	14.515137672	3.170408487
9.668236732	1.109306097	3.184067249
7.674949646	4.511047363	3.146596909
5.386029243	8.054596901	3.588571310

3.839870214 10.917425156 2.723735571

1.937836409 14.480265617 3.115542650

13.532526970 1.112675548 3.186541319

11.594147682 4.472555161 3.178398609

9.600019455 7.847356319 3.149560213

7.746990681 11.161338806 3.092918873

5.779880047 14.466289520 3.145424128

17.416582108 1.111060381 3.219564676

15.472874641 4.473476410 3.186832190

13.542969704 7.822370529 3.184367895

11.609027863 11.169136047 3.155673504

9.669171333 14.529059410 3.154605627

3.811608076 8.965897560 2.720506907

3.983142138 8.857475281 5.860367775

5.115412235 8.202944756 5.239686966

3.039819002 8.395097733 5.561193943

3.951293707 9.927455902 5.591765404

4.114473820 8.763484001 6.946804047

CH2OH ads BSi

1.0

19.3415393829 0.0000000000 0.0000000000

-9.6707696915 16.7502644539 0.0000000000

0.0000000000 0.0000000000 20.0017776489

Si B C O H

49 1 1 1 3

Cartesian

0.011541550 2.266608953 3.604513645

-1.910078645 5.589731216 3.585022926

-3.825362206 8.928699493 3.613620043

-5.798710346 12.277028084 3.596994162

-7.741093159 15.638280869 3.591016293

3.869830370 2.252158403 3.574156046

1.968240499 5.719645977 3.398487091

0.103324965	8.902605057	3.389781952
-1.907072306	12.267042160	3.591081142
-3.860420942	15.632633209	3.596667767
7.741135597	2.235699892	3.574543476
5.820223331	5.610467911	3.249239922
2.011177540	12.212035179	3.383924484
0.023716141	15.600892067	3.614844084
11.615512848	2.225730896	3.611380816
9.671162605	5.582376957	3.592078447
7.706027985	8.911316872	3.319858074
5.696374416	12.194324493	3.391471624
3.872331142	15.611554146	3.584135532
15.478544235	2.230360508	3.603170395
13.551376343	5.578359604	3.611742020
11.603096008	8.925450325	3.570272923
9.655599594	12.277920723	3.574135303
7.716152668	15.610779762	3.606012344
1.932797551	1.128913760	3.163780212
0.040484414	4.512304783	3.166402102
-1.885704398	7.815621853	3.154080391
-3.851468563	11.159978867	3.160555601
-5.802118301	14.516674995	3.155369759
5.801306248	1.122479558	3.147183180
3.875519514	4.484435081	3.121326447
2.119034052	7.947068214	2.955747366
0.013879670	11.158381462	3.138087988
-1.919842124	14.504605293	3.161037207
9.684720039	1.091073155	3.166418791
7.761951447	4.464369774	3.031733274
5.598652840	7.922171593	3.396788120
3.843555212	10.947020531	2.932750702
1.956687808	14.478634834	3.152966976
13.545727730	1.102755427	3.150927544
11.609744072	4.464454651	3.147286654

9.672847748 7.798189163 3.049299240

7.720175743 11.158588409 3.130442381

5.783730507 14.466903687 3.164792299

17.418773651 1.112467647 3.172522306

15.490060806 4.467980862 3.151090145

13.569993019 7.817332268 3.163993120

11.598067284 11.164532661 3.149415255

9.661318779 14.516443253 3.160893202

3.812009573 8.974070549 3.485175371

3.969362497 8.919813156 5.134220600

5.150681019 7.942210674 5.268343449

3.132769585 8.454855919 5.671996117

4.233678341 9.872940063 5.590420723

5.804689884 8.134480476 5.976520061

O ads BSi

1.0

19.3415393829 0.0000000000 0.0000000000

-9.6707696915 16.7502644539 0.0000000000

0.0000000000 0.0000000000 20.0017776489

Si B O

49 1 1

Cartesian

0.006664788 2.258839846 3.591470718

-1.916108966 5.584434509 3.570840597

-3.863420963 8.937406540 3.603745222

-5.820934772 12.283095360 3.608350277

-7.736977100 15.632466316 3.592979431

3.859146357 2.253267527 3.592809677

1.946234703 5.708630085 3.643135071

-0.019915398 8.958784103 3.382890224

-1.965384007 12.299433708 3.593590975

-3.877239227 15.647369385 3.608874798

7.747838020 2.240376234 3.523339033

5.862090111	5.439963818	3.653098106
1.899082899	12.285705566	3.388425589
-0.002034537	15.625392914	3.604407787
11.609489441	2.226601601	3.606473446
9.673584938	5.578750610	3.547663450
7.892848969	8.950849533	3.658630371
5.697639942	12.208168030	3.652135849
3.875670195	15.614956856	3.572525501
15.480270386	2.228592873	3.603600502
13.545398712	5.581712723	3.607000828
11.603922844	8.918642044	3.526391506
9.647092819	12.279306412	3.595636368
7.716930866	15.612894058	3.591567516
1.928496957	1.118856311	3.152804136
0.052440435	4.511685371	3.167697430
-1.954386473	7.809076309	3.098702431
-3.891271114	11.167329788	3.149536848
-5.803626537	14.517014503	3.149560452
5.797715187	1.126466751	3.135186911
3.831471205	4.497997284	3.201038122
2.004381895	7.977487564	3.295482635
-0.067072555	11.203156471	3.067193031
-1.946553707	14.533628464	3.150040865
9.678708076	1.101268411	3.151867867
7.784118176	4.446164131	2.956214905
6.040117741	7.679884911	3.741536140
3.762675285	11.025884628	3.286104441
1.929332018	14.535840034	3.100551844
13.547553062	1.109084368	3.173659086
11.614844322	4.459591389	3.148781300
9.713142395	7.782266617	2.959997177
7.688659668	11.180274010	3.207249165
5.788730621	14.445431709	3.168699503
17.411947250	1.112981200	3.160278320

15.482080460 4.461970806 3.175184727

13.554648399 7.816275120 3.152503967

11.591796875 11.163869858 3.135906219

9.665192604 14.518019676 3.151016474

3.609643936 9.084408760 3.770794153

4.712668896 8.452425957 4.333146572

OH ads BSi

1.0

19.3415393829 0.0000000000 0.0000000000

-9.6707696915 16.7502644539 0.0000000000

0.0000000000 0.0000000000 20.0017776489

Si B O H

49 1 1 1

Cartesian

0.001788639 2.250051022 3.591881990

-1.930253267 5.583926678 3.590689182

-3.858655453 8.927763939 3.592930555

-5.801850319 12.275429726 3.591703176

-7.743421078 15.637301445 3.590835810

3.866619587 2.244973183 3.578697920

1.945972323 5.681922913 3.537862062

0.081999749 8.900349617 3.520833015

-1.923777699 12.277343750 3.581140518

-3.860973120 15.636988640 3.591776848

7.733779430 2.254161358 3.586218596

5.787872791 5.657247066 3.552801132

2.001521111 12.234059334 3.519849777

0.009197631 15.629324913 3.592825651

11.603827477 2.233351231 3.596280336

9.669385910 5.584795952 3.602807283

7.661774635 8.905552864 3.551270008

5.723238468 12.225997925 3.537861109

3.870107651 15.630867958 3.591942549

15.474334717	2.232848167	3.594422340
13.538500786	5.584459782	3.596389055
11.585556984	8.925460815	3.586432219
9.658392906	12.277893066	3.578239918
7.722467422	15.623311043	3.591584921
1.929046154	1.124103665	3.155843735
0.022234904	4.496932983	3.181314707
-1.905376196	7.818084717	3.183449507
-3.863612890	11.159642220	3.157895327
-5.802397728	14.516903877	3.160339832
5.806080818	1.125033498	3.157382727
3.864880323	4.484525204	3.181183815
2.103369236	7.923937321	3.091833830
0.010411233	11.161478043	3.182886362
-1.925506115	14.516299248	3.158198595
9.666109085	1.118461609	3.160320759
7.716937065	4.500960350	3.172656536
5.662515640	7.893352509	3.064615726
3.857025623	10.978656769	3.076411963
1.946819901	14.494201660	3.184380531
13.538513184	1.115445375	3.154577255
11.602044106	4.468316555	3.151515484
9.629990578	7.817743301	3.173654318
7.717500687	11.158397675	3.181116104
5.787024498	14.482002258	3.181485415
17.411075592	1.114345670	3.161448240
15.473837852	4.467834473	3.155107975
13.535877228	7.820066452	3.160207510
11.599315643	11.159346581	3.157415867
9.661273003	14.517129898	3.155876637
3.899261475	8.925127983	3.531947613
4.261729240	8.767084122	4.939553261
3.581961870	9.014850616	5.566122055

CH ads BSi

1.0

19.3415393829	0.0000000000	0.0000000000
-9.6707696915	16.7502644539	0.0000000000
0.0000000000	0.0000000000	20.0017776489

Si	B	C	H
49	1	1	1

Cartesian

0.004905732	2.254901886	3.585827351
-1.929381013	5.583534241	3.595937252
-3.850692511	8.931052208	3.592664003
-5.799455643	12.278635025	3.594324589
-7.738774300	15.634782791	3.590568781
3.869472504	2.222689629	3.598042011
1.966769218	5.668162823	3.594126701
0.062992439	8.909563065	3.535106659
-1.931084871	12.281805038	3.587574244
-3.862622261	15.633554459	3.594497681
7.737547398	2.225109339	3.595683336
5.793316364	5.605069637	3.506882429
1.987598896	12.240413666	3.539221525
0.010823479	15.620109558	3.592510700
11.603816986	2.232615709	3.594898701
9.664338112	5.586740494	3.582936287
7.720883846	8.932451248	3.496772766
5.745573521	12.211678505	3.595022917
3.870517015	15.628882408	3.596040487
15.475604057	2.231969595	3.594095469
13.539158821	5.584597111	3.594630718
11.614988327	8.937616348	3.596962214
9.681974411	12.288550377	3.598352432
7.720389843	15.618161201	3.585299015
1.928642273	1.117554307	3.157972813
0.028852647	4.506592274	3.176538229

-1.911391854 7.814094067 3.165360928

-3.864395857 11.162086487 3.157385826

-5.799083233 14.514951706 3.154117584

5.804954529 1.113850236 3.146485090

3.868187904 4.458341599 3.169799328

2.091036797 7.921086788 3.132081032

0.002844520 11.166190147 3.193224192

-1.928056479 14.516004562 3.157598019

9.674876213 1.105054617 3.163991928

7.725491524 4.463867664 3.125698566

5.683824539 7.888935566 3.216521740

3.856504440 10.979154587 3.124649763

1.947538614 14.497413635 3.166301966

13.538619995 1.113971353 3.156726360

11.598389626 4.470376015 3.164354801

9.673983574 7.826372623 3.122290373

7.745842457 11.174295425 3.168715715

5.782560825 14.470623016 3.176504374

17.412429810 1.113583684 3.159075499

15.475211143 4.468332767 3.156855345

13.552268982 7.819072723 3.164665937

11.609117508 11.166371346 3.146058321

9.667466164 14.521183968 3.158071280

3.745858908 9.004881859 3.532361746

4.644752026 8.496281624 4.612160683

4.646000862 8.517420769 5.707330227

CH2 ads BSi

1.0

19.3415393829 0.0000000000 0.0000000000

-9.6707696915 16.7502644539 0.0000000000

0.0000000000 0.0000000000 20.0017776489

Si B C H

49 1 1 2

Cartesian

0.004089843	2.254336834	3.588923216
-1.935139060	5.581609249	3.602449417
-3.850724459	8.933570862	3.605981588
-5.796233654	12.282307625	3.594250441
-7.736383915	15.633433342	3.589814663
3.869956970	2.235519409	3.601269722
1.964307785	5.697942734	3.529453993
0.078706011	8.897220612	3.470251560
-1.930595517	12.281765938	3.588814259
-3.864372969	15.629064560	3.594346285
7.731253624	2.237771749	3.599264622
5.787897110	5.623579025	3.438583136
2.005985498	12.233091354	3.471952200
0.008998593	15.617881775	3.606079578
11.608664513	2.233339310	3.598964930
9.652819633	5.594188213	3.564961910
7.690581799	8.924861908	3.447598457
5.722306728	12.202428818	3.533183336
3.869007826	15.636049271	3.602712870
15.472758293	2.233707190	3.590862989
13.541165352	5.580269337	3.599086285
11.596606255	8.935467720	3.598181248
9.670133591	12.280578613	3.600579739
7.722046375	15.621639252	3.589236498
1.931119442	1.118304253	3.161081553
0.033407133	4.510739803	3.180308580
-1.906652093	7.813576221	3.158305645
-3.866319895	11.164851189	3.157164335
-5.798038483	14.514263153	3.156822681
5.804301739	1.110728264	3.141540289
3.863975525	4.470652580	3.171619177
2.093558073	7.929764748	3.042181015
0.010676013	11.161085129	3.176902294

-1.931471109 14.516488075 3.157202959

9.675079346 1.110282779 3.164281845

7.716720581 4.470199108 3.104546070

5.621506214 7.918568134 3.246683359

3.853728771 10.969454765 3.054466486

1.950850606 14.494235992 3.158266783

13.539952278 1.120374441 3.155406952

11.601235390 4.469058990 3.165291548

9.653947830 7.833404064 3.107063055

7.732138634 11.166455269 3.172230959

5.781961918 14.468665123 3.179499865

17.409399033 1.116885543 3.163449764

15.470857620 4.464293480 3.155395985

13.545868874 7.816311836 3.164022446

11.611409187 11.168030739 3.142012596

9.668144226 14.518595695 3.160814285

3.727105618 9.011191368 3.537348509

4.577602863 8.501943588 4.758820057

5.114644051 9.242724419 5.361377239

4.206494331 7.663134575 5.339928627

CH3 ads BSi

1.0

19.3415393829 0.0000000000 0.0000000000

-9.6707696915 16.7502644539 0.0000000000

0.0000000000 0.0000000000 20.0017776489

Si B C H

49 1 1 3

Cartesian

0.007148653 2.265189648 3.597800732

-1.922962785 5.589908600 3.592936039

-3.837213039 8.923604965 3.597886801

-5.803434849 12.277911186 3.579096794

-7.741843700 15.635877609 3.579128504

3.868417740	2.276865721	3.580557585
1.958340764	5.716215611	3.398976564
0.127649516	8.887922287	3.398915052
-1.896766305	12.261988640	3.580909014
-3.863888264	15.636413574	3.578881025
7.728256702	2.267270088	3.597463131
5.778078079	5.715435028	3.391795874
2.036426783	12.195747375	3.392856359
0.025067847	15.609929085	3.597957373
11.609921455	2.236641169	3.599389315
9.658639908	5.590443134	3.591179132
7.609624863	8.888213158	3.390330315
5.699149609	12.195566177	3.391126871
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13.538422585	5.577610016	3.599132776
11.570443153	8.923701286	3.596897840
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7.710874557	15.608613014	3.597129822
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-3.853414774	11.161933899	3.165137529
-5.802720547	14.516803741	3.168752670
5.799108982	1.132778525	3.164925337
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13.539060593 1.109850645 3.152688265

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CO@SiAl

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Si Al C O

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-7.737389565 15.634027481 3.596503019

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CHO@SiAl

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Si Al C O H

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COH@SiAl

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Si Al C O H

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CH2O@SiAl

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Si Al C O H

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CHOH@SiAl

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Si Al C O H

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-0.028930314	8.895813942	3.507342100
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-3.861095190	15.627575874	3.606911182
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Si Al C O H

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Si Al C O H

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Si Al C H

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