Supplementary Information

Atomic coordinates and absolute energies of all optimized structures in ″A Reversible Switch for Hydrogen Adsorption and Desorption: Electric Fields″

1. H_2/Li_8/SWCN Bridge site F = 0.000 au

Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	13.162349	9.882012	1.404023
2	C	13.162028	9.883810	5.664084
3	C	13.162106	9.883874	2.811171
4	C	13.162306	9.882108	7.071241
5	C	12.903194	11.108132	3.534744
6	C	12.902255	11.105985	7.794903
7	C	12.902200	11.105875	0.680406
8	C	12.903118	11.108034	4.940517
9	C	12.218244	12.135351	1.410489
10	C	12.223170	12.140949	5.670276
11	C	12.223686	12.141352	2.805082
12	C	12.218485	12.135690	7.064921
13	C	11.168700	12.786981	3.533371
14	C	11.166774	12.783930	7.794329
15	C	11.166812	12.784050	0.680989
16	C	11.168464	12.786512	4.941991
17	C	9.940624	13.021551	1.404408
18	C	9.942071	13.025377	5.663120
19	C	9.941978	13.024913	2.812175
20	C	9.940660	13.021665	7.070980
21	C	8.716158	12.769089	3.535403
22	C	8.714442	12.772225	7.794535
23	C	8.714527	12.772094	0.680796
24	C	8.716203	12.769213	4.939925
25	C	7.680110	12.095694	1.410449
26	C	7.687203	12.088602	5.670026
27	C	7.686710	12.088931	2.805423
28	C	7.679551	12.096320	7.065039
29	C	7.028069	11.042185	3.534969
30	C	7.026648	11.046280	7.794572
31	C	7.026680	11.046139	0.680755
32	C	7.028202	11.042123	4.940423
33	C	6.798851	9.814841	1.404397
34	C	6.798730	9.812486	5.664563

35	C	6.798687	9.812491	2.810816
36	C	6.798882	9.814936	7.070957
37	C	7.056509	8.587899	3.534689
38	C	7.059588	8.591607	7.794835
39	C	7.059506	8.591493	0.680498
40	C	7.056545	8.587905	4.940676
41	C	7.741231	7.560885	1.410507
42	C	7.734435	7.553888	5.670019
43	C	7.734734	7.554195	2.805252
44	C	7.741534	7.561219	7.064756
45	C	8.784986	6.901907	3.534601
46	C	8.788379	6.904824	7.794711
47	C	8.788321	6.904750	0.680628
48	C	8.784991	6.901931	4.940781
49	C	10.017571	6.672815	1.404149
50	C	10.015590	6.672637	5.664169
51	C	10.015534	6.672600	2.811167
52	C	10.017567	6.672809	7.071177
53	C	11.239669	6.930052	3.534762
54	C	11.242968	6.927705	7.794607
55	C	11.243051	6.927621	0.680706
56	C	11.239784	6.929968	4.940545
57	C	12.279408	7.601489	1.410028
58	C	12.273138	7.607511	5.670428
59	C	12.272604	7.608037	2.804722
60	C	12.278927	7.601954	7.065131
61	C	12.930630	8.654022	3.534680
62	C	12.932852	8.651371	7.794507
63	C	12.932970	8.651233	0.680733
64	C	12.930727	8.653890	4.940579
65	Li	9.938692	14.533032	4.236824
66	Li	14.640837	9.895365	8.497611
67	Li	5.319347	9.804469	8.497662
68	Li	5.318858	9.805881	4.237731
69	Li	14.640521	9.893805	4.237657
70	Li	10.025668	5.192145	4.237666
71	Li	10.033227	5.192595	8.497659
72	Li	9.924784	14.513216	8.497883
73	H	11.447335	15.781563	4.218524
74	H	11.719060	15.039618	4.216042

	Total Energy	Energy change	Max Gradient	Max Displacement
opt==	-2478.6115645	-0.0000095	0.001183	0.013384

2. H_2/Li_8/SWCN Bridge site *F* = +0.010 au

Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	13.205352	9.803740	1.398441
2	C	13.266530	9.808774	5.657996
3	C	13.204990	9.803230	2.809402
4	C	13.266898	9.809275	7.069969
5	C	13.061924	11.042036	3.524917
6	C	13.069319	11.038226	7.785562
7	C	13.062579	11.043292	0.683238
8	C	13.069121	11.037335	4.941999
9	C	12.299160	12.040531	1.407408
10	C	12.305527	12.024376	5.665067
11	C	12.297478	12.038367	2.800257
12	C	12.306685	12.025731	7.062832
13	C	11.194578	12.609693	3.531869
14	C	11.198714	12.603287	7.791419
15	C	11.196930	12.613067	0.675502
16	C	11.196531	12.600198	4.936732
17	C	9.962458	12.828732	1.400313
18	C	9.961952	12.812093	5.659839
19	C	9.961851	12.830403	2.808153
20	C	9.962642	12.810858	7.067118
21	C	8.724609	12.615566	3.533025
22	C	8.724900	12.605431	7.791792
23	C	8.726468	12.614994	0.675278
24	C	8.722999	12.605849	4.935218
25	C	7.630418	12.030047	1.407535
26	C	7.624019	12.013453	5.664291
27	C	7.630567	12.029494	2.800533
28	C	7.624282	12.013978	7.062711
29	C	6.885465	11.017471	3.524735
30	C	6.882246	11.011608	7.785675
31	C	6.886761	11.017610	0.682849
32	C	6.880833	11.011156	4.941721
33	C	6.780607	9.774695	1.398287
34	C	6.713739	9.777963	5.657596
35	C	6.781019	9.774661	2.809209
36	C	6.715748	9.778303	7.069882
37	C	7.086333	8.598748	3.531208
38	C	7.065112	8.600704	7.786550
39	C	7.086621	8.598874	0.676463

40	C	7.063463	8.600063	4.941105
41	C	7.772670	7.598443	1.400577
42	C	7.762505	7.604797	5.660743
43	C	7.772681	7.598500	2.807164
44	C	7.763344	7.605307	7.066793
45	C	8.798077	6.920991	3.530895
46	C	8.796645	6.930683	7.789342
47	C	8.798110	6.920872	0.676843
48	C	8.796353	6.930715	4.938385
49	C	10.015201	6.659709	1.396806
50	C	10.014912	6.677723	5.657250
51	C	10.015169	6.659686	2.810973
52	C	10.015110	6.677775	7.070523
53	C	11.231578	6.924855	3.531062
54	C	11.233007	6.934878	7.789531
55	C	11.231546	6.925363	0.676720
56	C	11.232839	6.934520	4.938312
57	C	12.251890	7.611164	1.400555
58	C	12.261219	7.617096	5.660932
59	C	12.252230	7.610315	2.807221
60	C	12.261413	7.617484	7.067004
61	C	12.924345	8.620613	3.531327
62	C	12.945488	8.623544	7.786790
63	C	12.924664	8.621301	0.676488
64	C	12.944755	8.623079	4.941066
65	Li	9.963112	14.373816	4.244585
66	Li	15.339627	10.950935	0.654081
67	Li	4.603220	10.746454	0.641037
68	Li	4.601201	10.745154	3.563838
69	Li	15.345947	10.915245	3.574987
70	Li	10.013732	5.121815	4.242662
71	Li	10.014143	5.121948	8.485165
72	Li	9.966385	14.365648	8.483334
73	H	11.507097	15.673137	4.255989
74	H	11.772172	14.938007	4.251612

	Total Energy	Energy change	Max Gradient	Max Displacement
opt==	-2479.0370743	-0.0000058	0.000614	0.024378

3. H_2/Li_8/SWCN Bridge site F = –0.010 au

Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	14.110402	9.994168	1.375460
2	C	14.108708	9.993978	5.637429
3	C	14.110999	9.993344	2.847869
4	C	14.107182	9.994654	7.107081
5	C	13.380232	11.069665	3.543353
6	C	13.381409	11.070583	7.801238
7	C	13.379240	11.071226	0.680923
8	C	13.381097	11.068166	4.942749
9	C	12.337432	11.682374	1.408147
10	C	12.335568	11.679268	5.667031
11	C	12.336599	11.678590	2.815931
12	C	12.336822	11.683390	7.077083
13	C	11.156768	11.998247	3.530109
14	C	11.158569	12.013495	7.789648
15	C	11.159828	12.010856	0.694202
16	C	11.155904	12.002427	4.953836
17	C	9.929736	12.108862	1.399068
18	C	9.928731	12.110578	5.659757
19	C	9.928876	12.105794	2.825499
20	C	9.929662	12.111574	7.083459
21	C	8.700052	12.004547	3.530363
22	C	8.701778	12.002456	7.789775
23	C	8.701287	12.001644	0.693874
24	C	8.700096	12.006228	4.954409
25	C	7.529051	11.651665	1.408700
26	C	7.529046	11.651799	5.667425
27	C	7.528913	11.652300	2.815528
28	C	7.530066	11.649249	7.076724
29	C	6.509790	11.001803	3.544072
30	C	6.508786	10.999190	7.802247
31	C	6.508519	11.002981	0.680433
32	C	6.507698	11.000619	4.942434
33	C	5.841582	9.883577	1.375828
34	C	5.837558	9.883362	5.634744
35	C	5.842022	9.883902	2.848645
36	C	5.836587	9.883053	7.109694
37	C	6.490267	8.728096	3.529956
38	C	6.488971	8.728715	7.791317
39	C	6.490269	8.727667	0.694451
40	C	6.488796	8.728128	4.953040
41	C	7.565091	8.100515	1.409014
42	C	7.564635	8.102441	5.670472

43	C	7.566298	8.103182	2.815071
44	C	7.565573	8.105279	7.073572
45	C	8.778578	7.852702	3.533584
46	C	8.778429	7.856275	7.793906
47	C	8.778058	7.851977	0.690978
48	C	8.777985	7.856161	4.950673
49	C	10.025914	7.775959	1.408357
50	C	10.026154	7.783475	5.667107
51	C	10.026181	7.776119	2.815892
52	C	10.026331	7.783650	7.077185
53	C	11.273232	7.862199	3.533607
54	C	11.272877	7.865843	7.793717
55	C	11.272787	7.862591	0.690719
56	C	11.272748	7.865862	4.950533
57	C	12.480779	8.135744	1.410272
58	C	12.482042	8.136387	5.671485
59	C	12.481691	8.133386	2.814337
60	C	12.482851	8.134545	7.072981
61	C	13.534550	8.799590	3.530158
62	C	13.537111	8.799190	7.792498
63	C	13.533463	8.800563	0.693883
64	C	13.537385	8.798945	4.951899
65	Li	9.957687	13.740076	4.221062
66	Li	15.426600	9.028879	8.509457
67	Li	4.596948	8.845471	8.500739
68	Li	4.596137	8.845118	4.243882
69	Li	15.429584	9.026823	4.239171
70	Li	10.035360	6.173111	4.258695
71	Li	10.035562	6.170859	8.482997
72	Li	9.921923	13.731951	8.516169
73	H	11.367802	15.189468	4.034792
74	H	11.747710	14.515152	4.083176

	Total Energy	Energy change	Max Gradient	Max Displacement
opt==	-2479.1040591	-0.0000082	0.001782	0.007262

4. H_2/Li_8/SWCN Middle site F = 0.000 au

Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	13.174050	9.865433	1.404018

2	C	13.176543	9.864696	5.663979
3	C	13.174505	9.865178	2.810742
4	C	13.176146	9.864929	7.070812
5	C	12.924629	11.090182	3.534604
6	C	12.925609	11.090759	7.794770
7	C	12.924848	11.091095	0.680258
8	C	12.925272	11.089840	4.939892
9	C	12.250040	12.128852	1.409724
10	C	12.250182	12.124896	5.670409
11	C	12.246726	12.125424	2.804511
12	C	12.253585	12.128265	7.064844
13	C	11.198242	12.780497	3.534228
14	C	11.200295	12.780054	7.793895
15	C	11.199451	12.781887	0.680631
16	C	11.199155	12.778997	4.940699
17	C	9.969920	13.006696	1.404313
18	C	9.969692	12.993034	5.664043
19	C	9.969632	13.006919	2.810384
20	C	9.969971	12.991782	7.070704
21	C	8.743408	12.766299	3.534170
22	C	8.742982	12.763737	7.794032
23	C	8.743885	12.765464	0.680519
24	C	8.742457	12.764862	4.940718
25	C	7.702667	12.098347	1.409972
26	C	7.699973	12.096856	5.670480
27	C	7.703326	12.097547	2.804461
28	C	7.698916	12.097959	7.064619
29	C	7.038214	11.053700	3.534325
30	C	7.037195	11.053586	7.794594
31	C	7.037957	11.053932	0.680390
32	C	7.037586	11.053260	4.940192
33	C	6.803346	9.825185	1.403949
34	C	6.801251	9.824512	5.663911
35	C	6.803416	9.825103	2.810803
36	C	6.801163	9.824649	7.070873
37	C	7.060074	8.601365	3.534675
38	C	7.059745	8.601484	7.794843
39	C	7.060030	8.601467	0.680013
40	C	7.059747	8.601320	4.939997
41	C	7.735542	7.565857	1.409793
42	C	7.735520	7.566165	5.670107
43	C	7.735623	7.566028	2.804699
44	C	7.735549	7.566119	7.064937
45	C	8.780841	6.905451	3.534577

46	C	8.781405	6.906637	7.794677
47	C	8.781442	6.906517	0.680120
48	C	8.780776	6.905538	4.940209
49	C	10.008760	6.668116	1.403996
50	C	10.008703	6.668567	5.664000
51	C	10.008720	6.667908	2.810872
52	C	10.008754	6.668772	7.070727
53	C	11.233019	6.921170	3.534679
54	C	11.233906	6.920156	7.794581
55	C	11.233869	6.920049	0.680230
56	C	11.233042	6.921286	4.940113
57	C	12.271194	7.593509	1.409978
58	C	12.269324	7.595405	5.670297
59	C	12.269358	7.595153	2.804545
60	C	12.271187	7.593728	7.064780
61	C	12.933839	8.638071	3.534556
62	C	12.933692	8.638047	7.794561
63	C	12.933460	8.638027	0.680292
64	C	12.934047	8.638102	4.940165
65	Li	9.950300	14.518327	4.248267
66	Li	14.676186	9.866262	8.498711
67	Li	5.300361	9.851148	8.498746
68	Li	5.300640	9.849527	4.236049
69	Li	14.676729	9.862722	4.236114
70	Li	10.002050	5.165335	4.237713
71	Li	10.038540	5.166558	8.497092
72	Li	9.974125	14.517905	8.485347
73	H	9.972625	15.962455	6.390071
74	H	9.970746	15.167041	6.379172

	Total Energy	Energy change	Max Gradient	Max Displacement
opt==	-2478.6099125	-0.0000199	0.002023	0.020924

5. H_2/Li_8/SWCN Middle site F = +0.010 au

Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	13.214389	9.832438	1.411048
2	C	13.279676	9.838614	5.670416
3	C	13.214298	9.832533	2.821985
4	C	13.279443	9.838591	7.082838

5	C	13.058794	11.070126	3.537072
6	C	13.068835	11.065111	7.799038
7	C	13.059129	11.070007	0.695774
8	C	13.070148	11.065590	4.954320
9	C	12.286016	12.059388	1.419779
10	C	12.297996	12.045168	5.677763
11	C	12.285744	12.059544	2.812806
12	C	12.296897	12.045356	7.075073
13	C	11.180424	12.625491	3.544278
14	C	11.183628	12.613751	7.803464
15	C	11.180343	12.623477	0.687780
16	C	11.182477	12.610365	4.948874
17	C	9.941971	12.820169	1.413197
18	C	9.942851	12.781306	5.671657
19	C	9.941813	12.820062	2.819700
20	C	9.942841	12.798494	7.079396
21	C	8.704692	12.617252	3.544177
22	C	8.702923	12.605020	7.803614
23	C	8.704863	12.614896	0.687965
24	C	8.703875	12.602514	4.948669
25	C	7.606971	12.032855	1.419877
26	C	7.599019	12.015706	5.677619
27	C	7.607051	12.033325	2.812816
28	C	7.600251	12.015595	7.075171
29	C	6.866609	11.017383	3.537388
30	C	6.863925	11.009094	7.799352
31	C	6.866682	11.016987	0.695505
32	C	6.862423	11.009725	4.954000
33	C	6.778896	9.772763	1.411123
34	C	6.711472	9.774591	5.670477
35	C	6.779289	9.773083	2.822086
36	C	6.711421	9.774363	7.082826
37	C	7.099476	8.601363	3.544303
38	C	7.075183	8.600471	7.798967
39	C	7.098686	8.600887	0.689016
40	C	7.076574	8.601613	4.954321
41	C	7.792523	7.605963	1.413404
42	C	7.782030	7.610882	5.673445
43	C	7.792586	7.606052	2.819965
44	C	7.782087	7.611032	7.079670
45	C	8.821707	6.934571	3.543468
46	C	8.819948	6.944029	7.802033
47	C	8.821608	6.934533	0.689911
48	C	8.819965	6.944109	4.951317

49	C	10.039677	6.677473	1.409381
50	C	10.039449	6.695936	5.669721
51	C	10.039699	6.677760	2.824101
52	C	10.039458	6.696242	7.083644
53	C	11.255034	6.946647	3.543754
54	C	11.256446	6.956853	7.802031
55	C	11.255033	6.946624	0.689607
56	C	11.256418	6.956988	4.951295
57	C	12.273642	7.634772	1.413405
58	C	12.282830	7.641965	5.673621
59	C	12.273603	7.634980	2.819889
60	C	12.282892	7.641848	7.079516
61	C	12.941617	8.648237	3.544419
62	C	12.963017	8.650614	7.799355
63	C	12.941284	8.648226	0.688704
64	C	12.962443	8.651250	4.953886
65	Li	9.942157	14.371844	4.271379
66	Li	15.335587	10.948227	9.176424
67	Li	4.558731	10.631312	9.186991
68	Li	4.558607	10.642750	3.571761
69	Li	15.333302	10.962249	3.582806
70	Li	10.043392	5.133212	4.255953
71	Li	10.040292	5.133179	8.497740
72	Li	9.933306	14.361539	-0.017538
73	H	10.002335	15.715586	5.908477
74	H	9.978237	14.954701	6.122616

	Total Energy	Energy change	Max Gradient	Max Displacement
opt==	-2479.0365066	-0.0000197	0.000634	0.043164

6. H_2/Li_8/SWCN Middle site $F = -0.010$ au

Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	14.085128	9.992946	1.372191
2	C	14.076452	9.999257	5.636421
3	C	14.082575	9.990671	2.842815
4	C	14.074247	9.997820	7.099123
5	C	13.365744	11.072931	3.538378
6	C	13.366398	11.076075	7.799800
7	C	13.373335	11.080648	0.679205

8	C	13.375858	11.085165	4.937522
9	C	12.339769	11.711738	1.404354
10	C	12.340832	11.712651	5.663544
11	C	12.339771	11.714653	2.812089
12	C	12.342445	11.719085	7.072343
13	C	11.166857	12.057681	3.524238
14	C	11.166694	12.053936	7.786673
15	C	11.167734	12.057467	0.691376
16	C	11.165028	12.047956	4.948417
17	C	9.936231	12.145351	1.396536
18	C	9.936369	12.142971	5.655130
19	C	9.935443	12.147708	2.819612
20	C	9.936613	12.150790	7.079410
21	C	8.709925	12.018545	3.526282
22	C	8.707682	12.026146	7.785012
23	C	8.710985	12.016099	0.689163
24	C	8.708124	12.022503	4.950161
25	C	7.545297	11.648027	1.403629
26	C	7.544499	11.645290	5.663561
27	C	7.542134	11.654988	2.812495
28	C	7.545036	11.645961	7.071775
29	C	6.532960	10.986756	3.539250
30	C	6.530169	10.988769	7.798064
31	C	6.532714	10.986037	0.676415
32	C	6.523665	10.995292	4.938109
33	C	5.860862	9.873575	1.371913
34	C	5.861643	9.873825	5.630555
35	C	5.860858	9.874143	2.843008
36	C	5.862086	9.872129	7.104445
37	C	6.493586	8.709453	3.524791
38	C	6.503430	8.716179	7.787548
39	C	6.493120	8.708482	0.689833
40	C	6.504280	8.719154	4.946831
41	C	7.569143	8.084606	1.405875
42	C	7.572417	8.080698	5.665674
43	C	7.569560	8.084990	2.808850
44	C	7.570870	8.076685	7.068747
45	C	8.780498	7.831384	3.530309
46	C	8.777190	7.800923	7.787601
47	C	8.779342	7.830186	0.684055
48	C	8.778106	7.802949	4.946635
49	C	10.022685	7.740998	1.403440
50	C	10.028238	7.742575	5.663007
51	C	10.023943	7.740775	2.811264

52	C	10.028007	7.742287	7.071429
53	C	11.274445	7.813445	3.526229
54	C	11.269674	7.847964	7.791324
55	C	11.271526	7.817327	0.687781
56	C	11.269318	7.848058	4.942580
57	C	12.471470	8.123842	1.406490
58	C	12.474314	8.126461	5.666507
59	C	12.478784	8.108734	2.808918
60	C	12.476445	8.120780	7.068085
61	C	13.512398	8.803169	3.529411
62	C	13.527711	8.794340	7.783753
63	C	13.509637	8.807976	0.684600
64	C	13.525478	8.797604	4.950422
65	Li	9.916267	13.765065	4.242131
66	Li	15.426964	9.007189	8.511410
67	Li	4.602629	8.840326	8.510917
68	Li	4.603217	8.840449	4.223771
69	Li	15.428917	8.999290	4.239404
70	Li	10.040691	6.134889	4.250572
71	Li	10.041489	6.134908	8.484593
72	Li	9.912558	13.760298	8.508427
73	H	9.961205	15.398592	5.716138
74	H	9.960208	14.677736	6.002081

	Total Energy	Energy change	Max Gradient	Max Displacement
opt==	-2479.1005756	0.0000522	0.004376	0.016226

7. H_2/Li_8/SWCN Atop site F = 0.000 au

Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	13.160224	9.871692	1.406877
2	C	13.159300	9.871849	5.666811
3	C	13.159420	9.871805	2.813886
4	C	13.159927	9.871839	7.073857
5	C	12.897514	11.095696	3.537606
6	C	12.898101	11.094990	7.797709
7	C	12.898084	11.094668	0.683100
8	C	12.897147	11.095532	4.943091
9	C	12.211417	12.122147	1.414057
10	C	12.216063	12.127573	5.673030

11	C	12.217424	12.128746	2.808159
12	C	12.212681	12.123629	7.067203
13	C	11.165937	12.779971	3.537816
14	C	11.164538	12.778477	7.797544
15	C	11.164169	12.777948	0.683113
16	C	11.165817	12.780176	4.943503
17	C	9.935864	13.008552	1.407251
18	C	9.936483	13.009264	5.666862
19	C	9.936509	13.008838	2.814380
20	C	9.935887	13.008416	7.073297
21	C	8.711435	12.755103	3.538055
22	C	8.710990	12.755795	7.797575
23	C	8.711290	12.755448	0.683074
24	C	8.711500	12.755170	4.943323
25	C	7.677119	12.078789	1.413366
26	C	7.676107	12.080635	5.673055
27	C	7.675073	12.081534	2.808045
28	C	7.676194	12.079756	7.067824
29	C	7.022403	11.030795	3.537446
30	C	7.022696	11.030154	7.797495
31	C	7.022733	11.029958	0.683403
32	C	7.022630	11.030674	4.943231
33	C	6.794809	9.799464	1.406939
34	C	6.794656	9.800095	5.666962
35	C	6.794660	9.800033	2.813788
36	C	6.795011	9.799538	7.073864
37	C	7.058435	8.576834	3.537678
38	C	7.057469	8.575950	7.797589
39	C	7.057594	8.576066	0.683135
40	C	7.058600	8.577027	4.943065
41	C	7.739745	7.545279	1.413308
42	C	7.742216	7.547661	5.673414
43	C	7.741247	7.546677	2.807561
44	C	7.738845	7.544348	7.067642
45	C	8.789846	6.892016	3.537507
46	C	8.788199	6.890782	7.797457
47	C	8.788378	6.890928	0.683242
48	C	8.790019	6.892174	4.943181
49	C	10.018124	6.659501	1.406737
50	C	10.019397	6.659693	5.666761
51	C	10.019374	6.659707	2.813932
52	C	10.018094	6.659523	7.073948
53	C	11.244621	6.914793	3.537408
54	C	11.242581	6.916063	7.797451

55	C	11.242485	6.916148	0.683216
56	C	11.244516	6.914884	4.943249
57	C	12.275917	7.593950	1.413618
58	C	12.281089	7.589001	5.672702
59	C	12.281807	7.588315	2.808160
60	C	12.276552	7.593319	7.067221
61	C	12.931564	8.640777	3.537390
62	C	12.931319	8.641878	7.797424
63	C	12.931238	8.641921	0.683227
64	C	12.931429	8.640911	4.943294
65	Li	9.954856	14.510595	4.230903
66	Li	14.658183	9.886614	8.500256
67	Li	5.297050	9.788966	8.500307
68	Li	5.297022	9.789697	4.240405
69	Li	14.657693	9.885103	4.240462
70	Li	10.026810	5.160592	4.240386
71	Li	10.036310	5.160756	8.500349
72	Li	9.924526	14.514122	8.503634
73	H	9.989443	16.406516	3.639974
74	H	9.990923	16.474516	4.413652

	Total Energy	Energy change	Max Gradient	Max Displacement
opt==	-2478.6062949	0.0000108	0.001758	0.034076

8. H_2/Li_8/SWCN Atop site F = +0.010 au

Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	13.220984	9.803787	1.406133
2	C	13.222252	9.803724	5.665970
3	C	13.220866	9.803698	2.817816
4	C	13.222372	9.803757	7.077718
5	C	13.065131	11.040879	3.533348
6	C	13.067404	11.041012	7.793489
7	C	13.066383	11.041064	0.690593
8	C	13.066379	11.041016	4.950334
9	C	12.308177	12.038021	1.414799
10	C	12.307740	12.037440	5.674668
11	C	12.306810	12.037699	2.809279
12	C	12.308257	12.037088	7.069096
13	C	11.200521	12.610889	3.539969

14	C	11.200502	12.606374	7.799720
15	C	11.200371	12.607081	0.684139
16	C	11.200798	12.609597	4.944327
17	C	9.960302	12.798453	1.408207
18	C	9.960126	12.797042	5.668933
19	C	9.960045	12.803870	2.815892
20	C	9.959967	12.793823	7.075337
21	C	8.724775	12.581155	3.540197
22	C	8.724929	12.575892	7.799872
23	C	8.725691	12.576790	0.684013
24	C	8.724920	12.578954	4.944292
25	C	7.628517	11.988721	1.414961
26	C	7.628119	11.988242	5.674797
27	C	7.627762	11.990927	2.809777
28	C	7.626041	11.989666	7.069612
29	C	6.876882	10.988384	3.532940
30	C	6.873584	10.988279	7.793236
31	C	6.875950	10.987760	0.691248
32	C	6.874674	10.988041	4.950793
33	C	6.727048	9.748780	1.406626
34	C	6.723895	9.748940	5.666483
35	C	6.727686	9.749310	2.817379
36	C	6.723846	9.748962	7.077525
37	C	7.050424	8.571782	3.536383
38	C	7.048326	8.571106	7.796113
39	C	7.049783	8.571281	0.687513
40	C	7.049105	8.571599	4.947723
41	C	7.741853	7.573740	1.408660
42	C	7.741367	7.573899	5.668677
43	C	7.742047	7.573838	2.815176
44	C	7.740991	7.573713	7.075167
45	C	8.776088	6.903512	3.538406
46	C	8.775759	6.903921	7.798297
47	C	8.775976	6.903596	0.685314
48	C	8.775905	6.903876	4.945537
49	C	9.995531	6.655860	1.404457
50	C	9.995490	6.656587	5.664536
51	C	9.995569	6.655948	2.819290
52	C	9.995438	6.656512	7.079207
53	C	11.209969	6.928159	3.538229
54	C	11.209992	6.928184	7.798056
55	C	11.209858	6.928092	0.685540
56	C	11.210106	6.928260	4.945694
57	C	12.231405	7.616069	1.408813

58	C	12.232489	7.615410	5.668898
59	C	12.231656	7.615956	2.814844
60	C	12.232315	7.615446	7.075010
61	C	12.910017	8.623256	3.536309
62	C	12.909624	8.623684	7.796137
63	C	12.909325	8.623673	0.687472
64	C	12.910409	8.623267	4.947689
65	Li	9.945145	14.331466	4.241390
66	Li	15.301460	10.906416	8.504696
67	Li	4.686544	10.962913	8.512367
68	Li	4.687591	10.964788	4.231344
69	Li	15.296746	10.914234	4.238378
70	Li	10.018245	5.114521	4.242322
71	Li	10.019501	5.114363	8.501491
72	Li	9.948712	14.328240	8.502192
73	H	9.969067	16.203523	3.590619
74	H	10.015790	16.342543	4.345977

	Total Energy	Energy change	Max Gradient	Max Displacement
opt==	-2479.0223664	-0.0000133	0.000720	0.011232

9. H_2/Li_8/SWCN Atop site F = –0.010 au

Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	14.118805	9.986003	1.372867
2	C	14.117537	9.984032	5.632364
3	C	14.117366	9.984028	2.845064
4	C	14.118949	9.986034	7.104614
5	C	13.390233	11.062349	3.539246
6	C	13.390788	11.063699	7.799284
7	C	13.390652	11.063627	0.678257
8	C	13.390545	11.062540	4.938262
9	C	12.344383	11.670891	1.404840
10	C	12.342464	11.666047	5.664686
11	C	12.342629	11.666773	2.812822
12	C	12.345253	11.672187	7.072669
13	C	11.163352	11.990549	3.526582
14	C	11.164511	11.991709	7.786344
15	C	11.164166	11.991882	0.690952
16	C	11.163272	11.990235	4.950908

17	C	9.933935	12.080631	1.395711
18	C	9.933285	12.081407	5.655765
19	C	9.933454	12.082201	2.821697
20	C	9.934295	12.079399	7.081623
21	C	8.705401	11.967348	3.526617
22	C	8.707044	11.961632	7.786639
23	C	8.706411	11.962956	0.690889
24	C	8.704945	11.967800	4.951003
25	C	7.533813	11.613633	1.404460
26	C	7.532020	11.618452	5.664374
27	C	7.533689	11.614955	2.812760
28	C	7.535780	11.609078	7.072595
29	C	6.510128	10.969758	3.539170
30	C	6.508317	10.970270	7.799015
31	C	6.509425	10.969578	0.678044
32	C	6.511419	10.968625	4.937856
33	C	5.834965	9.855892	1.372069
34	C	5.835045	9.856057	5.632049
35	C	5.835006	9.856269	2.845449
36	C	5.834529	9.855932	7.105495
37	C	6.481638	8.698701	3.527556
38	C	6.481366	8.698251	7.787545
39	C	6.481315	8.697944	0.690123
40	C	6.481482	8.698358	4.950108
41	C	7.562812	8.082029	1.406992
42	C	7.563196	8.082914	5.667030
43	C	7.563327	8.083265	2.810592
44	C	7.562926	8.082477	7.070624
45	C	8.777060	7.838910	3.530388
46	C	8.776643	7.838140	7.790370
47	C	8.776613	7.838011	0.687247
48	C	8.777011	7.838861	4.947217
49	C	10.024550	7.772284	1.404556
50	C	10.025004	7.772213	5.664380
51	C	10.025016	7.772142	2.813173
52	C	10.024532	7.772378	7.072993
53	C	11.271718	7.859681	3.530172
54	C	11.270633	7.862140	7.790272
55	C	11.270674	7.862034	0.687271
56	C	11.271723	7.859706	4.947355
57	C	12.479456	8.133362	1.406821
58	C	12.481405	8.127639	5.666930
59	C	12.481347	8.127741	2.810543
60	C	12.479304	8.133715	7.070646

61	C	13.533856	8.793454	3.527623
62	C	13.533418	8.797217	7.787631
63	C	13.533448	8.797094	0.689849
64	C	13.533851	8.793496	4.949831
65	Li	9.923440	13.684350	4.238028
66	Li	15.428490	8.995162	8.498752
67	Li	4.585747	8.815726	8.498889
68	Li	4.585619	8.816530	4.238711
69	Li	15.427258	9.007548	4.238681
70	Li	10.041802	6.162528	4.238798
71	Li	10.043570	6.163101	8.498720
72	Li	9.914916	13.695547	8.497157
73	H	9.978004	15.603086	3.733930
74	H	9.981385	15.640135	4.501731

	Total Energy	Energy change	Max Gradient	Max Displacement
opt==	-2479.1004840	-0.0000079	0.001591	0.025697

10. H_2/Li/SWCN Bridge site *F* = 0.000 au

Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	13.063730	9.939503	1.407012
2	C	13.067308	9.938303	5.667090
3	C	13.067199	9.938072	2.821026
4	C	13.063878	9.939716	7.081092
5	C	12.827720	11.145299	3.536922
6	C	12.823507	11.145927	7.797862
7	C	12.823331	11.145762	0.690147
8	C	12.827993	11.145470	4.951234
9	C	12.169328	12.190089	1.408477
10	C	12.179976	12.190136	5.674315
11	C	12.179181	12.189345	2.813757
12	C	12.170039	12.190905	7.079585
13	C	11.170634	12.899673	3.541502
14	C	11.164463	12.912343	7.802843
15	C	11.164194	12.911748	0.685165
16	C	11.171187	12.900140	4.946248
17	C	9.950182	13.160412	1.405177
18	C	9.949846	13.158599	5.678059
19	C	9.949548	13.158739	2.809967

20	C	9.950320	13.160929	7.082800
21	C	8.735405	12.870517	3.542080
22	C	8.742729	12.881422	7.802612
23	C	8.742774	12.881199	0.685350
24	C	8.735581	12.870213	4.946088
25	C	7.753624	12.138971	1.408105
26	C	7.745414	12.136921	5.673529
27	C	7.745276	12.136870	2.814670
28	C	7.753634	12.139207	7.080003
29	C	7.111996	11.084134	3.536575
30	C	7.114643	11.085202	7.797575
31	C	7.114832	11.085077	0.690612
32	C	7.112577	11.083932	4.951531
33	C	6.893505	9.874562	1.407035
34	C	6.892701	9.873324	5.667055
35	C	6.892053	9.873224	2.821086
36	C	6.894128	9.874774	7.081170
37	C	7.124292	8.664302	3.537884
38	C	7.123164	8.664558	7.797868
39	C	7.123233	8.664388	0.690341
40	C	7.124553	8.664379	4.950296
41	C	7.788396	7.627838	1.408260
42	C	7.790173	7.629208	5.668071
43	C	7.790008	7.629016	2.819979
44	C	7.789611	7.629223	7.079883
45	C	8.803175	6.928837	3.538939
46	C	8.802441	6.928275	7.798908
47	C	8.802109	6.927524	0.689208
48	C	8.803529	6.929867	4.949183
49	C	10.012052	6.687144	1.409286
50	C	10.012429	6.689337	5.669289
51	C	10.012404	6.688344	2.818781
52	C	10.012247	6.688845	7.078798
53	C	11.216725	6.953805	3.538648
54	C	11.216234	6.954124	7.798641
55	C	11.216094	6.954013	0.689456
56	C	11.216424	6.954641	4.949393
57	C	12.214163	7.675773	1.408009
58	C	12.214238	7.676075	5.667818
59	C	12.214619	7.675386	2.820281
60	C	12.214247	7.676106	7.080106
61	C	12.859498	8.724589	3.537623
62	C	12.856940	8.725928	7.797702
63	C	12.856736	8.725877	0.690402

64	C	12.859276	8.724795	4.950451
65	Li	9.970879	14.752079	4.243224
66	H	11.670803	15.654094	4.264846
67	H	11.230256	16.289602	4.237973

	Total Energy	Energy change	Max Gradient	Max Displacement
opt==	-2426.8416293	-0.0000180	0.001149	0.016111

11. H_2/Li/SWCN Bridge site *F* = +0.010 au

Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	13.221606	9.950912	1.404711
2	C	13.214840	9.948024	5.664723
3	C	13.219844	9.948944	2.822767
4	C	13.212908	9.949976	7.082173
5	C	12.984183	11.156524	3.533917
6	C	12.970452	11.156358	7.794685
7	C	12.972459	11.156500	0.692457
8	C	12.976353	11.154054	4.952749
9	C	12.234140	12.160909	1.411586
10	C	12.245011	12.163680	5.675896
11	C	12.243679	12.159991	2.811493
12	C	12.234148	12.162894	7.075942
13	C	11.163771	12.773967	3.541940
14	C	11.160280	12.796689	7.803598
15	C	11.159431	12.791990	0.683690
16	C	11.163832	12.775786	4.945806
17	C	9.935308	12.994007	1.403628
18	C	9.934198	12.989255	5.678472
19	C	9.934479	12.987700	2.809457
20	C	9.934662	12.997403	7.084339
21	C	8.708131	12.749090	3.542434
22	C	8.715867	12.763517	7.803830
23	C	8.717151	12.759909	0.683766
24	C	8.707978	12.750167	4.945538
25	C	7.656144	12.106425	1.411882
26	C	7.644946	12.109162	5.675949
27	C	7.645966	12.106523	2.811671
28	C	7.654908	12.109193	7.076192
29	C	6.937978	11.079910	3.534431

30	C	6.942789	11.084489	7.794752
31	C	6.943051	11.083199	0.692965
32	C	6.943170	11.079076	4.953036
33	C	6.736588	9.869779	1.405208
34	C	6.737067	9.867775	5.665253
35	C	6.730167	9.867192	2.823218
36	C	6.737192	9.870700	7.082706
37	C	7.007811	8.674376	3.541731
38	C	7.020374	8.680581	7.801963
39	C	7.017492	8.679538	0.685880
40	C	7.012634	8.675747	4.946165
41	C	7.755450	7.700949	1.407117
42	C	7.755842	7.699333	5.666977
43	C	7.754802	7.700964	2.821167
44	C	7.757060	7.700130	7.080962
45	C	8.810154	7.079560	3.535664
46	C	8.810182	7.074624	7.795582
47	C	8.808660	7.075121	0.692515
48	C	8.813058	7.082838	4.952139
49	C	10.020945	6.868885	1.408913
50	C	10.022319	6.858341	5.668456
51	C	10.021684	6.867417	2.819819
52	C	10.021686	6.856753	7.079866
53	C	11.231437	7.095846	3.535426
54	C	11.227745	7.102459	7.795610
55	C	11.226790	7.106062	0.691902
56	C	11.230044	7.097819	4.952334
57	C	12.265928	7.753643	1.407156
58	C	12.269289	7.746750	5.666457
59	C	12.267526	7.750883	2.821457
60	C	12.267118	7.750342	7.080785
61	C	12.984198	8.747173	3.541532
62	C	12.980713	8.748868	7.801290
63	C	12.978718	8.751423	0.685979
64	C	12.978891	8.747894	4.945792
65	Li	9.932417	14.592433	4.244522
66	H	11.729349	15.304349	4.262290
67	H	11.400392	16.005857	4.250593

	Total Energy	Energy change	Max Gradient	Max Displacement
opt==	-2427.2911807	0.0000116	0.002064	0.012639

12. H_2/SWCN Atop site F = 0.000 au

Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	13.142605	9.829254	1.400004
2	C	13.144166	9.828714	5.660029
3	C	13.141289	9.828564	2.813682
4	C	13.143824	9.829140	7.073785
5	C	12.893472	11.034394	3.530054
6	C	12.896458	11.036193	7.789994
7	C	12.896650	11.036547	0.683808
8	C	12.895050	11.034920	4.943749
9	C	12.208144	12.057711	1.400052
10	C	12.206011	12.054905	5.660001
11	C	12.205846	12.055091	2.813779
12	C	12.207285	12.056476	7.073667
13	C	11.180523	12.735992	3.530426
14	C	11.181859	12.738560	7.790084
15	C	11.182441	12.740063	0.683760
16	C	11.180711	12.736226	4.943302
17	C	9.972272	12.974300	1.400040
18	C	9.971874	12.975228	5.659696
19	C	9.971869	12.974576	2.814020
20	C	9.972297	12.973825	7.073708
21	C	8.765181	12.723771	3.530450
22	C	8.765942	12.723867	7.790067
23	C	8.765469	12.725032	0.683747
24	C	8.765343	12.723149	4.943310
25	C	7.748121	12.030749	1.400060
26	C	7.747660	12.030364	5.659932
27	C	7.748359	12.030006	2.813844
28	C	7.748909	12.029692	7.073653
29	C	7.071621	11.001569	3.530017
30	C	7.072380	11.001490	7.790014
31	C	7.071947	11.001875	0.683835
32	C	7.069984	11.002125	4.943848
33	C	6.837209	9.792770	1.400029
34	C	6.835845	9.792710	5.660021
35	C	6.838224	9.792597	2.813713
36	C	6.836924	9.792673	7.073786
37	C	7.081667	8.585344	3.530152
38	C	7.080831	8.585243	7.790140
39	C	7.080754	8.585236	0.683716

40	C	7.080329	8.585146	4.943720
41	C	7.769725	7.564366	1.400120
42	C	7.769758	7.564619	5.660129
43	C	7.769775	7.564038	2.813704
44	C	7.770070	7.564800	7.073696
45	C	8.797488	6.885300	3.530054
46	C	8.797746	6.886451	7.790074
47	C	8.797651	6.886230	0.683763
48	C	8.797647	6.886244	4.943752
49	C	10.007165	6.653198	1.400046
50	C	10.007267	6.653551	5.660002
51	C	10.007240	6.652563	2.813858
52	C	10.007208	6.653849	7.073806
53	C	11.214225	6.899419	3.530065
54	C	11.213816	6.900959	7.790091
55	C	11.213820	6.900805	0.683749
56	C	11.214070	6.900304	4.943738
57	C	12.233478	7.590961	1.400095
58	C	12.234114	7.590497	5.660100
59	C	12.233782	7.590249	2.813730
60	C	12.233342	7.591298	7.073703
61	C	12.911077	8.618664	3.530072
62	C	12.910794	8.619628	7.790101
63	C	12.910646	8.619655	0.683686
64	C	12.911889	8.618663	4.943811
65	H	9.943595	15.472139	3.842402
66	H	9.942556	15.482450	4.611337

	Total Energy	Energy change	Max Gradient	Max Displacement
opt==	-2419.4196707	-0.0000118	0.000367	0.010782

13. H_2/SWCN Atop site F = +0.010 au

Coordinates (Angstroms)

	ATOM	X	Y	Z
1	C	13.282425	9.822135	1.397716
2	C	13.287049	9.822182	5.657551
3	C	13.284340	9.822080	2.815901
4	C	13.283461	9.822355	7.075805
5	C	13.049799	11.030740	3.528107
6	C	13.048518	11.030778	7.788133

7	C	13.048598	11.030888	0.685344
8	C	13.051555	11.031242	4.945408
9	C	12.286730	12.019426	1.405140
10	C	12.287151	12.018202	5.664973
11	C	12.287174	12.019140	2.808486
12	C	12.287678	12.020379	7.068270
13	C	11.187104	12.593838	3.529562
14	C	11.187384	12.596229	7.789175
15	C	11.187692	12.597606	0.684103
16	C	11.187139	12.593138	4.943778
17	C	9.969028	12.777156	1.393015
18	C	9.968912	12.772018	5.652767
19	C	9.969019	12.776269	2.820583
20	C	9.968909	12.776948	7.080239
21	C	8.751591	12.589898	3.529581
22	C	8.750463	12.594831	7.789145
23	C	8.750425	12.595591	0.684066
24	C	8.751437	12.588772	4.943626
25	C	7.655635	12.008188	1.405201
26	C	7.654146	12.007607	5.665004
27	C	7.654718	12.008383	2.808298
28	C	7.654259	12.009276	7.068034
29	C	6.907795	11.006916	3.528145
30	C	6.910596	11.006208	7.788180
31	C	6.911087	11.006163	0.685245
32	C	6.904079	11.008106	4.945424
33	C	6.701745	9.793340	1.397721
34	C	6.696438	9.793626	5.657412
35	C	6.699757	9.793505	2.815974
36	C	6.698806	9.793623	7.075780
37	C	6.985762	8.604428	3.534348
38	C	6.986418	8.604511	7.794269
39	C	6.986582	8.604126	0.679288
40	C	6.984162	8.604312	4.939435
41	C	7.736893	7.633071	1.399747
42	C	7.737091	7.635176	5.659845
43	C	7.736710	7.633513	2.813938
44	C	7.736746	7.633903	7.073901
45	C	8.797528	7.021324	3.528306
46	C	8.797334	7.020488	7.788295
47	C	8.797004	7.018893	0.685449
48	C	8.797722	7.022836	4.945371
49	C	10.008677	6.802865	1.401005
50	C	10.008680	6.807580	5.661105

51	C	10.008755	6.804456	2.812657
52	C	10.008675	6.806045	7.072647
53	C	11.218607	7.029127	3.528378
54	C	11.218799	7.028088	7.788352
55	C	11.219016	7.026713	0.685410
56	C	11.218441	7.030286	4.945304
57	C	12.273900	7.649900	1.399764
58	C	12.273861	7.651618	5.659749
59	C	12.274458	7.650088	2.814010
60	C	12.274306	7.650225	7.073965
61	C	13.016291	8.628187	3.534274
62	C	13.014561	8.628737	7.794339
63	C	13.014064	8.628689	0.679291
64	C	13.017096	8.628246	4.939353
65	H	9.959175	15.400094	3.847042
66	H	9.957332	15.412679	4.615653

	Total Energy	Energy change	Max Gradient	Max Displacement
opt==	-2419.8724683	-0.0000029	0.000657	0.013998