

# Structural stability and electronic properties of $SP^3$ type silicon nanotubes

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## Supplementary Material

### Convergence Test

To check for convergence of the electronic structure calculations with respect to the size of the basis set we have performed comparative calculations for the SiNT [100] system. Table S1 presents the bandgap of this system as calculated using the 6-31G\*\* and 6-311G\* basis sets. As can be seen, for all functional approximations considered the bandgaps calculated using the two basis sets are converged to within less than 1.5%.

Functional	Band Gap [eV]		
	6-31G**	6-311G**	$\Delta$ [%]
LDA	2.943	2.985	1.42
PBE	3.067	3.074	0.21
HSE	3.880	3.895	0.36

Table S1: Bandgap of SiNT [100] as calculated using the LDA, PBE and HSE exchange-correlation functional approximations with the 6-31G\*\* and 6-311G\* atomic centered Gaussian basis sets.

### Consistency tests

As a part of the consistency test of our calculations we have presented in the main text comparisons of our LDA calculated bandgaps for SiNWs with reference values from the literature. Here, we present similar comparisons for the PBE and HSE functional approximations. In Fig. S1 PBE calculated bandgaps from existing literature are presented along with values obtained in the present study. Similarly, in Fig. S2 calculated bandgaps from existing literature using various hybrid functional approximations are presented along with values obtained in the present study using the HSE screened-exchange functional. As can be seen, our calculations for both functional approximations fit well within the trends previously reported for SiNWs thus reaffirming the validity of our calculations.

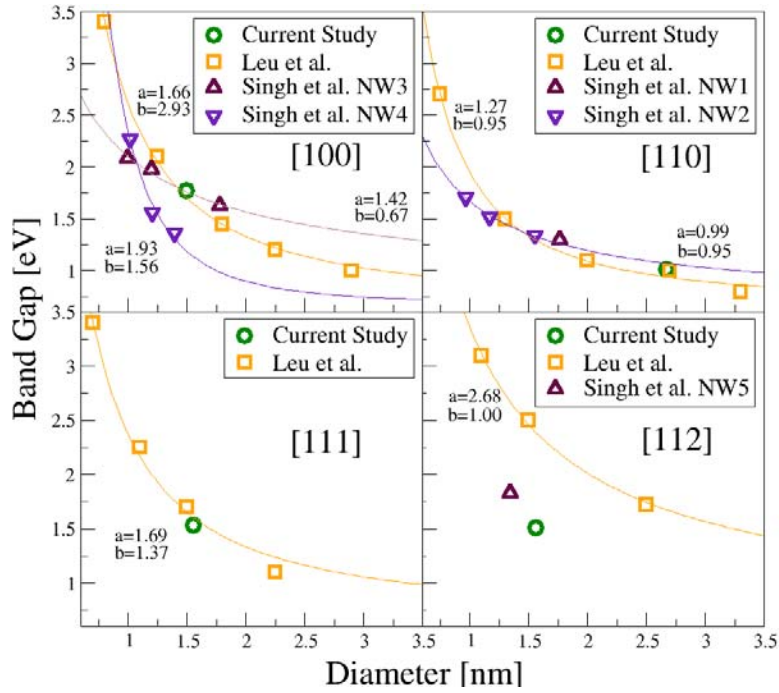


Figure S1: Comparison between PBE bandgaps obtained for SiNWs of different growth orientations and reference values. Full lines are added as guide to the eye using the same fitting procedure described in Fig. 3 of the main text. The obtained optimal fitting parameters are presented next to their corresponding fitting curve.

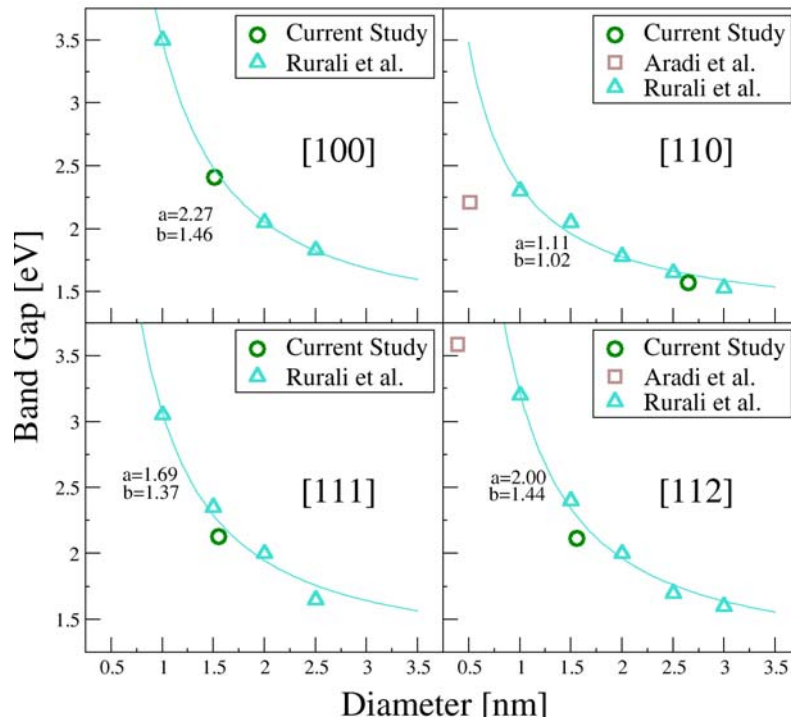


Figure S2: Comparison between HSE bandgaps obtained for SiNWs of different growth orientations and reference values. Full lines are added as guide to the eye using the same fitting procedure described in Fig. 3 of the main text. The obtained optimal fitting parameters are presented next to their corresponding fitting curve.

## Stability analysis

For completeness, we present a comparative view of the stability analysis results obtained using Eq. 1 of the main text and the three exchange-correlation functional approximations considered. Results presented for the HSE functional approximation match those given in Fig. 2 of the main text. All functional approximations considered produce a similar qualitative picture with minor quantitative differences. As stated in the main text, the PBE functional tends to predict a slightly lower stability (higher  $\delta G$  values) when compared to the predictions of the other functional approximations considered.

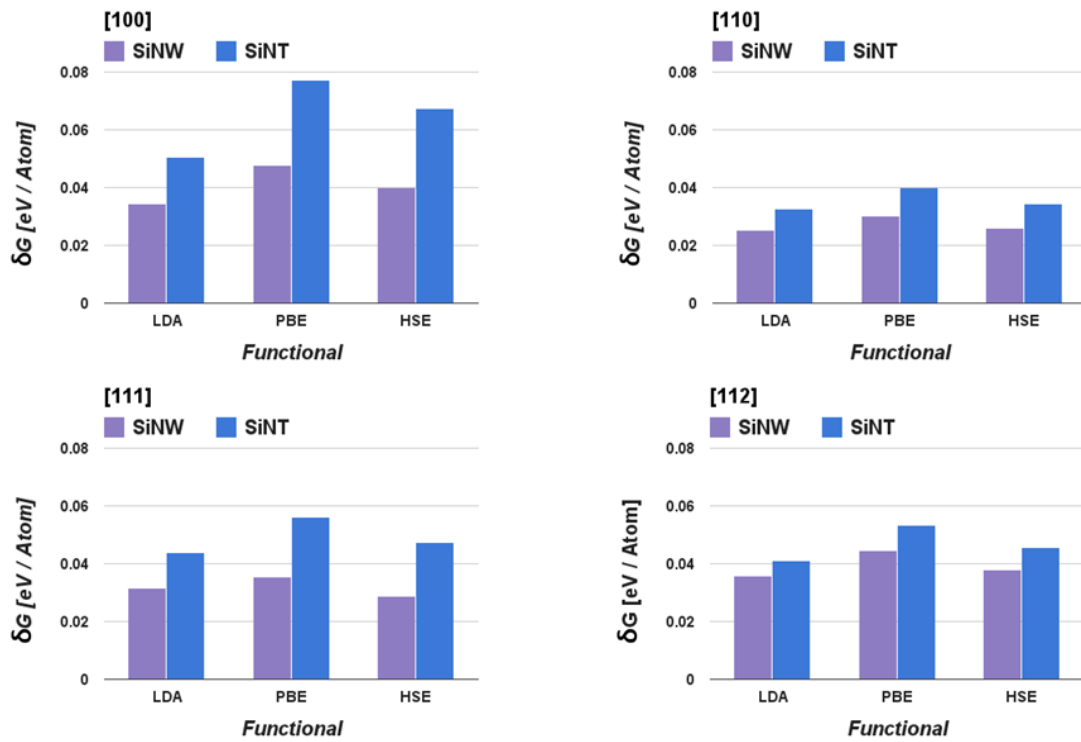


Figure S3: Comparison between  $\delta G$  values obtained using the LDA, PBE, and HSE functional approximations for the [100] (upper left panel), [110] (upper right panel), [111] (lower left panel), and [112] (lower right panel) SiNWs and SiNTs considered.

## Bandgap analysis

For completeness, we present a comparative view of the bandgap results obtained using the three exchange-correlation functional approximations considered. Results presented for the HSE functional approximation match those given in Fig. 4 of the main text. As may be expected the HSE screened hybrid exchange-correlation density functional predicts higher bandgap values than those obtained using the LDA and PBE counterparts and generally speaking the PBE functional gives slightly larger values than those obtained using the LDA.

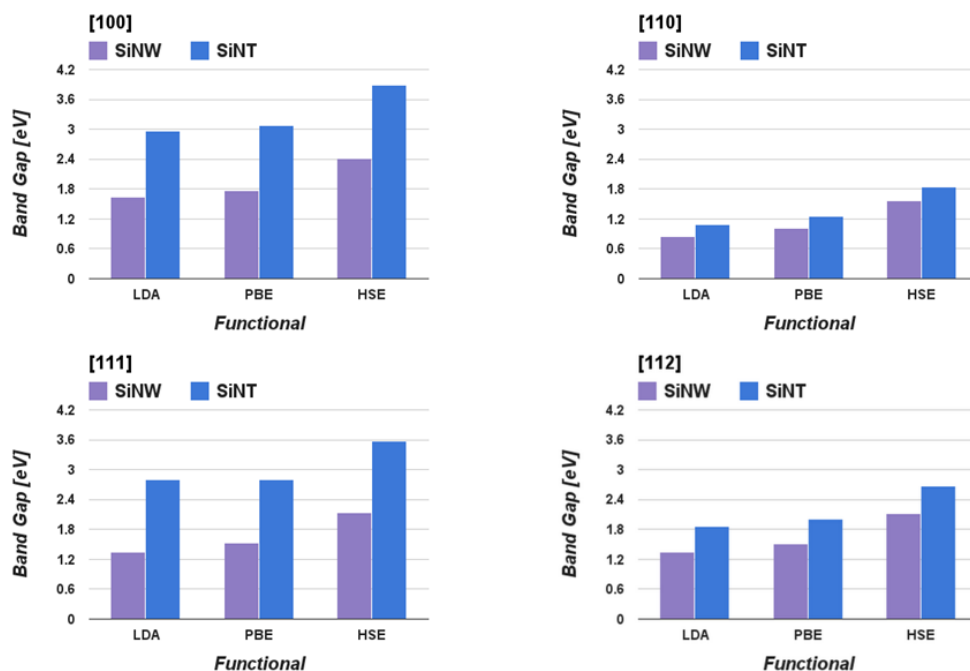


Figure S4: Comparison between bandgap values obtained using the LDA, PBE, and HSE functional approximations for the [100] (upper left panel), [110] (upper right panel), [111] (lower left panel), and [112] (lower right panel) SiNWs and SiNTs considered.

## Orbital structure

In Fig. 6 of the main text we have presented graphical representations of the CBM and VBM orbitals of the [110] SiNW and SiNT. Bellow, we present similar diagrams for all other systems considered in the present study. As stated in the main text, similar to the case of the [110] systems the orbitals in the SiNW systems tend to span the core region whereas in the SiNT counterparts the orbitals localize at the remaining outer shell of the system. Furthermore, here as well, the orbitals maintain their character in terms of general symmetry and nodal structure when going from the SiNW to the SiNT systems.

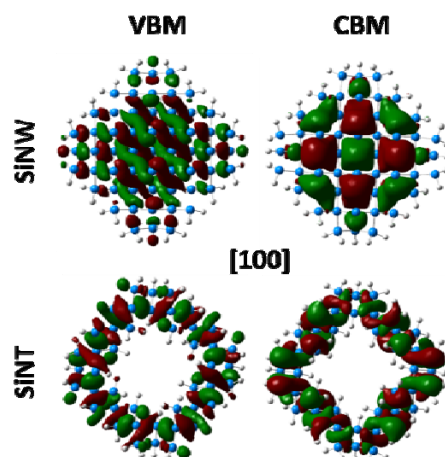


Fig. S5: VBM (left panels) and CBM (right panels) orbitals of the [100] SiNW (upper panels) and SiNT (lower panels). Obtained at the HSE/6-31G\*\* level of theory.

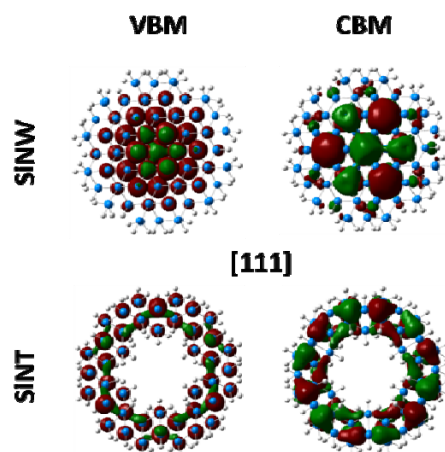


Fig. S6: VBM (left panels) and CBM (right panels) orbitals of the [111] SiNW (upper panels) and SiNT (lower panels). Obtained at the HSE/6-31G\*\* level of theory.

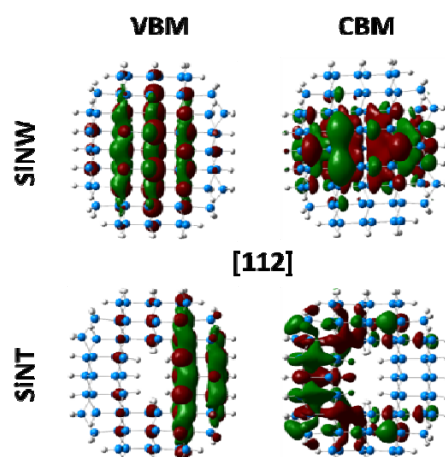


Fig. S7: VBM (left panels) and CBM (right panels) orbitals of the [112] SiNW (upper panels) and SiNT (lower panels). Obtained at the HSE/6-31G\*\* level of theory.

## Systems coordinates

Optimized coordinates (given in Å) of all SiNWs and SiNTs studied obtained using the LDA, PBE, and HSE functional approximations with the 6-31G<sup>\*\*</sup> atomic centered Gaussian basis set are presented below:

	Atomic Type	SiNT [100] - LDA			SiNT [100] - GGA			SiNT [100] - HSE		
		x	y	z	x	y	Z	x	y	z
1	Si	-2.384223	7.612490	-0.005821	-2.556220	7.727686	0.000000	-2.528993	7.676908	0.000000
2	Si	-2.204502	3.953461	3.904309	-2.417992	4.142047	4.076554	-2.375946	4.093936	4.035820
3	Si	-2.425664	0.005964	7.612258	-2.491399	-0.000058	7.727853	-2.479342	-0.000042	7.676856
4	Si	-2.603749	3.903796	-3.952447	-2.629643	4.076310	-4.142049	-2.632407	4.035806	-4.093913
5	Si	-2.603637	-3.902682	3.951397	-2.629653	-4.076338	4.141957	-2.632371	-4.035795	4.093822
6	Si	-2.201586	-3.952470	-3.904818	-2.417782	-4.141997	-4.076316	-2.375828	-4.093892	-4.035708
7	Si	-2.422507	-0.004878	-7.612713	-2.491238	-0.000072	-7.727910	-2.479306	-0.000018	-7.676877
8	Si	-2.381436	-7.611843	0.005010	-2.556173	-7.727875	-0.000007	-2.528949	-7.677003	-0.000023
9	Si	-0.848208	1.765073	7.479325	-0.869324	1.760626	7.830514	-0.891300	1.774591	7.725534
10	Si	-1.123681	6.044466	3.914061	-1.113462	6.132826	3.961786	-1.138932	6.113513	3.922520
11	Si	-1.172278	1.848522	3.802262	-1.200819	2.100202	4.125246	-1.189093	2.049288	4.055208
12	Si	-0.947226	-1.763865	8.116826	-0.995948	-1.815339	8.109322	-0.976489	-1.785098	8.094363
13	Si	-0.961243	5.766440	0.333950	-0.925457	5.953952	0.149125	-0.923297	5.905822	0.185992
14	Si	-1.027685	5.649251	-3.694668	-1.179548	5.955828	-3.852522	-1.122679	5.854894	-3.832206
15	Si	-0.953925	-2.226520	4.057556	-1.047357	-2.305432	4.175574	-1.035822	-2.294361	4.151464
16	Si	-1.027820	-5.648485	3.694765	-1.179545	-5.955851	3.852544	-1.122625	-5.854879	3.832233
17	Si	-0.953341	2.228206	-4.058173	-1.047203	2.305526	-4.175715	-1.035820	2.294409	-4.151561
18	Si	-0.959118	-5.765051	-0.333713	-0.925478	-5.954097	-0.149188	-0.923284	-5.905892	-0.186011
19	Si	-1.170164	-1.847126	-3.803100	-1.200707	-2.100099	-4.124985	-1.189005	-2.049235	-4.055060
20	Si	-0.944649	1.765482	-8.116983	-0.995874	1.815262	-8.109423	-0.976495	1.785063	-8.094428
21	Si	-0.844503	-1.763419	-7.479806	-0.869033	-1.760648	-7.830364	-0.891241	-1.774641	-7.725431
22	Si	-1.119631	-6.042875	-3.913361	-1.113208	-6.132747	-3.961776	-1.138795	-6.113463	-3.922494
23	Si	0.438406	1.689460	5.506446	0.431063	1.936355	5.852807	0.432873	1.884648	5.774029
24	Si	0.470157	6.113676	2.173852	0.410820	6.145670	2.122417	0.422729	6.127231	2.131598
25	Si	0.185524	2.173903	-6.112111	0.277464	2.122319	-6.145861	0.260166	2.131580	-6.127222
26	Si	0.216427	5.506210	-1.687463	0.257229	5.852524	-1.936330	0.250058	5.774023	-1.884640
27	Si	0.183567	-2.171785	6.112232	0.277324	-2.122344	6.145712	0.260152	-2.131583	6.127134
28	Si	0.217474	-5.505002	1.688418	0.257140	-5.852594	1.936282	0.250043	-5.774077	1.884618
29	Si	0.441360	-1.687562	-5.506485	0.431197	-1.936327	-5.852548	0.432921	-1.884624	-5.773915
30	Si	0.473715	-6.111245	-2.172648	0.410976	-6.145811	-2.122347	0.422844	-6.127277	-2.131554
31	Si	1.611635	-4.056793	-2.228023	1.735603	-4.175645	-2.305543	1.718829	-4.151609	-2.294301
32	Si	1.827948	-3.800647	1.847346	1.889036	-4.125041	2.100094	1.872017	-4.055258	2.049174
33	Si	1.615731	-0.332196	5.766543	1.613696	-0.149111	5.954100	1.606209	-0.185990	5.905756
34	Si	1.827470	3.802404	-1.846496	1.889074	4.124910	-2.100164	1.871997	4.055177	-2.049253
35	Si	1.779073	3.914267	-6.042453	1.801643	3.961759	-6.132827	1.821803	3.922526	-6.113486
36	Si	1.682569	3.696526	5.650509	1.867692	3.852651	5.956036	1.805536	3.832265	5.854890
37	Si	1.686335	-3.694130	-5.649783	1.867962	-3.852530	-5.955855	1.805680	-3.832180	-5.854800
38	Si	1.609047	4.059850	2.229287	1.735533	4.175564	2.305641	1.718740	4.151581	2.294382
39	Si	1.600629	8.118219	1.764809	1.684157	8.109216	1.815278	1.659382	8.094442	1.785055
40	Si	1.777931	-3.911417	6.042947	1.801614	-3.961697	6.132724	1.821850	-3.922472	6.113401

41	Si	1.604476	-8.115755	-1.764269	1.684279	-8.109397	-1.815323	1.659456	-8.094526	-1.785093
42	Si	1.503818	-7.478022	1.764416	1.557497	-7.830336	1.760619	1.574213	-7.725588	1.774594
43	Si	1.617884	0.334688	-5.765488	1.613869	0.149119	-5.954131	1.606243	0.186014	-5.905787
44	Si	1.502300	7.479467	-1.764078	1.557501	7.830304	-1.760652	1.574195	7.725552	-1.774634
45	H	-1.457130	8.791112	-0.278851	-1.741061	8.988971	-0.147150	-1.713115	8.921059	-0.173219
46	H	-3.352969	0.278966	8.790719	-3.306587	0.147113	8.989117	-3.295233	0.173185	8.920997
47	H	-3.349593	-0.278054	-8.791319	-3.306353	-0.147364	-8.989204	-3.295169	-0.173309	-8.921026
48	H	-1.453982	-8.790060	0.278607	-1.741031	-8.989145	0.147321	-1.713080	-8.921146	0.173277
49	H	0.121800	1.504917	8.625027	0.060070	1.312751	8.927589	0.009342	1.409267	8.861479
50	H	-1.442523	3.143959	7.680285	-1.442412	3.070429	8.282597	-1.495891	3.089491	8.072979
51	H	-0.609036	6.454511	5.279099	-0.373369	6.375849	5.243863	-0.494064	6.465264	5.217823
52	H	-2.235465	7.010130	3.535786	-2.062887	7.281324	3.805315	-2.139386	7.182863	3.654664
53	H	-0.747887	1.406577	2.417047	-0.746699	1.623992	2.777699	-0.746022	1.587739	2.711649
54	H	-2.346340	0.980774	4.224754	-2.268649	1.143337	4.557516	-2.264768	1.113768	4.478783
55	H	-1.555536	-2.977242	8.786574	-1.626931	-3.060520	8.655576	-1.581299	-3.004734	8.694536
56	H	0.104827	-1.168635	9.046016	-0.043711	-1.317043	9.163734	-0.011673	-1.242072	9.099584
57	H	-1.708673	4.524165	0.775465	-1.595919	4.637866	0.393451	-1.594934	4.608068	0.457634
58	H	-1.565788	7.055430	-3.865985	-1.961943	7.231531	-3.777707	-1.798412	7.179025	-3.895349
59	H	0.037749	5.446978	-4.760360	-0.275415	6.096152	-5.041829	-0.159909	5.827751	-4.969811
60	H	-1.308417	-0.834996	3.566432	-1.646553	-0.977474	3.828082	-1.578535	-0.961500	3.775648
61	H	0.150518	-2.713697	3.134717	-0.082497	-2.605750	3.068074	-0.051918	-2.632678	3.085974
62	H	-1.567166	-7.054346	3.864739	-1.961940	-7.231572	3.777884	-1.798331	-7.179015	3.895506
63	H	0.036678	-5.447475	4.761601	-0.275319	-6.096043	5.041800	-0.159817	-5.827623	4.969793
64	H	-1.307025	0.836398	-3.567298	-1.646195	0.977537	-3.827990	-1.578490	0.961553	-3.775670
65	H	0.150063	2.716072	-3.134425	-0.082294	2.606100	-3.068317	-0.051917	2.632797	-3.086095
66	H	-1.707118	-4.523469	-0.776364	-1.596045	-4.638094	-0.393685	-1.594976	-4.608167	-0.457715
67	H	-0.747142	-1.404347	-2.417715	-0.746607	-1.623775	-2.777474	-0.745915	-1.587664	-2.711517
68	H	-2.344339	-0.980181	-4.226998	-2.268563	-1.143297	-4.557315	-2.264684	-1.113729	-4.478633
69	H	-1.553574	2.978420	-8.786983	-1.626943	3.060423	-8.655602	-1.581354	3.004693	-8.694572
70	H	0.107654	1.170555	-9.046070	-0.043686	1.317022	-9.163905	-0.011696	1.242062	-9.099676
71	H	0.125693	-1.502415	-8.625161	0.060487	-1.312668	-8.927293	0.009437	-1.409337	-8.861351
72	H	-1.438097	-3.142532	-7.681285	-1.441965	-3.070459	-8.282618	-1.495821	-3.089548	-8.072877
73	H	-0.604482	-6.453112	-5.278137	-0.373081	-6.375422	-5.243898	-0.493918	-6.465106	-5.217819
74	H	-2.230969	-7.009005	-3.534989	-2.062609	-7.281299	-3.805581	-2.139251	-7.182835	-3.654732
75	H	0.507845	-3.133793	-2.716404	0.770653	-3.068293	-2.606149	0.734905	-3.086146	-2.632631
76	H	1.965718	-3.564803	-0.836688	2.334572	-3.827869	-0.977561	2.261514	-3.775766	-0.961431
77	H	3.002062	-4.223854	0.979963	2.956874	-4.557344	1.143264	2.947688	-4.478880	1.113665
78	H	1.403691	-2.415649	1.404573	1.434931	-2.777509	1.623834	1.428949	-2.711716	1.587572
79	H	2.364143	-0.774066	4.524938	2.284157	-0.393417	4.638001	2.277856	-0.457621	4.607999
80	H	3.001448	4.225374	-0.978900	2.956934	4.557162	-1.143336	2.947676	4.478759	-1.113752
81	H	1.403617	2.417045	-1.404434	1.434923	2.777392	-1.623905	1.428914	2.711638	-1.587668
82	H	2.891077	3.535833	-7.007815	2.751074	3.805552	-7.281357	2.822259	3.654738	-7.182857
83	H	1.264605	5.279276	-6.452854	1.061494	5.243860	-6.375557	1.176899	5.217830	-6.465171
84	H	0.617306	4.762432	5.448536	0.963385	5.041851	6.096110	0.842712	4.969818	5.827669
85	H	2.220350	3.867049	7.056909	2.650030	3.778130	7.231794	2.481237	3.895507	7.179030
86	H	0.621425	-4.760596	-5.449019	0.963846	-5.041845	-6.096194	0.842929	-4.969795	-5.827668
87	H	2.225700	-3.864154	-7.055641	2.650372	-3.777682	-7.231544	2.481417	-3.895294	-7.178930
88	H	0.505632	3.136202	2.717206	0.770719	3.068028	2.606006	0.734870	3.086052	2.632686

89	H	1.963371	3.568472	0.837850	2.334751	3.826039	0.977708	2.261466	3.775800	0.961519
90	H	0.548494	9.047018	1.169152	0.731961	9.163639	1.316929	0.694577	9.099666	1.242013
91	H	2.209129	8.788664	2.977700	2.315185	8.655521	3.060404	2.264213	8.694637	3.004672
92	H	2.889252	-3.532664	7.008990	2.751035	-3.805284	7.281249	2.822309	-3.654574	7.182734
93	H	1.264264	-5.276929	6.452656	1.061567	-5.243832	6.375623	1.177033	-5.217791	6.465176
94	H	0.552307	-9.044915	-1.169226	0.732074	-9.163869	-1.317103	0.694628	-9.099745	-1.242086
95	H	2.213348	-8.785587	-2.977316	2.315318	-8.655556	-3.060505	2.264265	-8.694677	-3.004740
96	H	2.097329	-7.679520	3.143559	2.130542	-8.282438	3.070441	2.178810	-8.073015	3.089496
97	H	0.533550	-8.623316	1.503389	0.628061	-8.927374	1.312746	0.673564	-8.861532	1.409295
98	H	2.365015	0.776927	-4.523252	2.284453	0.393611	-4.638134	2.277917	0.457736	-4.608068
99	H	2.096531	7.680158	-3.143027	2.130481	8.282512	-3.070458	2.178759	8.073029	-3.089538
100	H	0.531546	8.624685	-1.504440	0.628011	8.927270	-1.312704	0.673512	8.861458	-1.409294
101	Tv	5.463538	0.001088	0.001064	5.735824	0.000000	0.000000	5.691233	0.000000	0.000000

	Atomic Type	SiNW [100] - LDA			SiNW [100] - GGA			SiNW [100] - HSE		
		x	y	z	x	y	z	x	y	z
1	Si	-2.228503	5.404767	0.000000	-2.269321	5.465238	0.000000	-2.255451	5.436324	0.000000
2	Si	-2.257125	5.422237	-5.422274	-2.338055	5.483239	-5.483274	-2.320410	5.456811	-5.456846
3	Si	-2.199887	5.422250	5.422266	-2.200592	5.483252	5.483264	-2.190499	5.456825	5.456839
4	Si	-2.243206	2.708817	-2.708845	-2.291711	2.740628	-2.740653	-2.276145	2.726352	-2.726373
5	Si	-2.213802	2.708821	2.708847	-2.246933	2.740634	2.740659	-2.234763	2.726358	2.726374
6	Si	-2.228504	-0.000021	0.000005	-2.269322	-0.000020	0.000007	-2.255454	-0.000010	0.000003
7	Si	-2.228503	-0.000027	5.404799	-2.269323	-0.000020	5.465268	-2.255455	-0.000022	5.436344
8	Si	-2.228506	-0.000041	-5.404784	-2.269323	-0.000035	-5.465253	-2.255453	-0.000038	-5.436333
9	Si	-2.213807	-2.708868	-2.708827	-2.246937	-2.740673	-2.740639	-2.234768	-2.726388	-2.726356
10	Si	-2.243199	-2.708857	2.708845	-2.291707	-2.740662	2.740660	-2.276136	-2.726376	2.726372
11	Si	-2.199908	-5.422295	-5.422246	-2.200607	-5.483288	-5.483249	-2.190523	-5.456863	-5.456811
12	Si	-2.228506	-5.404817	0.000016	-2.269324	-5.465280	0.000015	-2.255456	-5.436353	0.000016
13	Si	-2.257094	-5.422273	5.422272	-2.338036	-5.483268	5.483275	-2.320383	-5.456840	5.456841
14	Si	-0.633427	6.737780	4.275987	-0.628993	6.822097	4.319244	-0.626151	6.789747	4.297877
15	Si	-0.952524	6.732061	-1.435527	-0.971351	6.808886	-1.444880	-0.966167	6.773837	-1.438855
16	Si	-0.891541	4.062857	-4.062899	-0.927951	4.114441	-4.114478	-0.920532	4.093657	-4.093695
17	Si	-0.633398	4.276009	6.737799	-0.628961	4.319272	6.822102	-0.626113	4.297908	6.789762
18	Si	-0.856209	4.068115	1.358542	-0.865173	4.118300	1.377453	-0.860680	4.096104	1.370127
19	Si	-0.869169	1.356444	-1.356470	-0.887132	1.373159	-1.373181	-0.881392	1.365787	-1.365805
20	Si	-0.952450	-1.435477	6.732108	-0.971275	-1.444816	6.808919	-0.966085	-1.438793	6.773872
21	Si	-0.869163	-1.356489	1.356472	-0.887127	-1.373199	1.373190	-0.881386	-1.365814	1.365804
22	Si	-0.856209	1.358511	4.068144	-0.865175	1.377428	4.118326	-0.860686	1.370108	4.096125
23	Si	-0.856211	-1.358577	-4.068132	-0.865175	-1.377482	-4.118313	-0.860683	-1.370157	-4.096113
24	Si	-0.952589	1.435539	-6.732077	-0.971390	1.444875	-6.808897	-0.966207	1.438846	-6.773853
25	Si	-0.891532	-4.062908	4.062888	-0.927946	-4.114481	4.114472	-0.920524	-4.093695	4.093680
26	Si	-0.856210	-4.068169	-1.358526	-0.865177	-4.118343	-1.377438	-0.860687	-4.096141	-1.370114
27	Si	-0.633466	-4.276006	-6.737784	-0.629015	-4.319267	-6.822093	-0.626182	-4.297900	-6.789741
28	Si	-0.633441	-6.737829	-4.275985	-0.628998	-6.822130	-4.319246	-0.626152	-6.789786	-4.297879
29	Si	-0.952530	-6.732117	1.435544	-0.971323	-6.808928	1.444865	-0.966139	-6.773879	1.438839
30	Si	0.510409	5.417264	2.718474	0.537578	5.481305	2.753451	0.531633	5.453052	2.738965
31	Si	0.486553	5.417260	-2.718483	0.477645	5.481299	-2.753459	0.477388	5.453049	-2.738975
32	Si	0.510401	2.718453	5.417295	0.537570	2.753433	5.481329	0.531622	2.738948	5.453075



33	Si	0.486558	2.718439	-5.417298	0.477650	2.753420	-5.481330	0.477393	2.738934	-5.453080
34	Si	0.498481	-2.711166	0.000005	0.507611	-2.743303	0.000008	0.504510	-2.728590	0.000004
35	Si	0.486554	-2.718498	5.417285	0.477646	-2.753463	5.481325	0.477393	-2.738981	5.453061
36	Si	0.498486	-0.000019	2.711145	0.507615	-0.000015	2.743290	0.504513	-0.000010	2.728576
37	Si	0.510406	-2.718513	-5.417276	0.537576	-2.753481	-5.481313	0.531627	-2.738999	-5.453054
38	Si	0.498476	-0.000026	-2.711142	0.507608	-0.000024	-2.743281	0.504504	-0.000018	-2.728574
39	Si	0.498480	2.711121	-0.000002	0.507611	2.743262	0.000002	0.504508	2.728559	-0.000004
40	Si	0.510400	-5.417319	-2.718465	0.537568	-5.481347	-2.753440	0.531618	-5.453090	-2.738951
41	Si	0.486563	-5.417310	2.718484	0.477654	-5.481338	2.753462	0.477401	-5.453078	2.738971
42	Si	1.630441	-4.275970	6.737806	1.644247	-4.319234	6.822113	1.635201	-4.297870	6.789763
43	Si	1.949456	6.732072	1.435488	1.986543	6.808896	1.444840	1.975157	6.773846	1.438816
44	Si	1.949505	-6.732115	-1.435529	1.986566	-6.808927	-1.444856	1.975173	-6.773878	-1.438824
45	Si	1.853170	1.358508	-4.068139	1.880396	1.377422	-4.118319	1.869701	1.370101	-4.096122
46	Si	1.630414	-6.737811	4.276004	1.644229	-6.822114	4.319269	1.635175	-6.789764	4.297903
47	Si	1.949403	-1.435481	-6.732095	1.986504	-1.444838	-6.808907	1.975115	-1.438819	-6.773860
48	Si	1.853170	-4.068158	1.358546	1.880399	-4.118334	1.377462	1.869704	-4.096128	1.370135
49	Si	1.888495	-4.062918	-4.062871	1.943168	-4.114492	-4.114454	1.929542	-4.093707	-4.093662
50	Si	1.853170	-1.358559	4.068144	1.880398	-1.377464	4.118328	1.869703	-1.370139	4.096121
51	Si	1.949579	1.435592	6.732080	1.986622	1.444907	6.808897	1.975227	1.438874	6.773856
52	Si	1.853172	4.068117	-1.358544	1.880396	4.118299	-1.377452	1.869700	4.096106	-1.370130
53	Si	1.630369	6.737771	-4.276017	1.644200	6.822087	-4.319271	1.635156	6.789739	-4.297904
54	Si	1.866125	-1.356489	-1.356462	1.902350	-1.373202	-1.373175	1.890406	-1.365815	-1.365798
55	Si	1.866129	1.356450	1.356472	1.902353	1.373166	1.373190	1.890409	1.365795	1.365805
56	Si	1.888500	4.062868	4.062896	1.943173	4.114451	4.114476	1.929549	4.093667	4.093692
57	Si	1.630353	4.275995	-6.737804	1.644178	4.319256	-6.822110	1.635136	4.297885	-6.789769
58	H	-1.397124	6.299656	-6.299689	-1.500285	6.368429	-6.368459	-1.487568	6.334516	-6.334550
59	H	-3.059889	6.299676	6.299674	-3.038359	6.368445	6.368442	-3.023339	6.334537	6.334536
60	H	-3.059924	-6.299699	-6.299663	-3.038383	-6.368466	-6.368431	-3.023377	-6.334562	-6.334520
61	H	-1.397079	-6.299678	6.299689	-1.500259	-6.368444	6.368458	-1.487528	-6.334543	6.334550
62	H	0.407189	7.123064	5.301171	0.389501	7.249478	5.342650	0.389142	7.202395	5.314770
63	H	-1.163524	8.014718	3.687124	-1.175897	8.084004	3.720816	-1.164517	8.045995	3.708678
64	H	-0.212590	7.804458	-0.683762	-0.235278	7.875188	-0.690649	-0.240037	7.838139	-0.694340
65	H	-1.899137	7.424452	-2.380230	-1.900182	7.525853	-2.377785	-1.893683	7.473000	-2.369470
66	H	-1.163443	3.687216	8.014789	-1.175809	3.720918	8.084051	-1.164421	3.708782	8.046073
67	H	0.407239	5.301206	7.122991	0.389550	5.342692	7.249393	0.389208	5.314819	7.202308
68	H	-1.898977	-2.380106	7.424720	-1.900013	-2.377635	7.526077	-1.893514	-2.369339	7.473261
69	H	-0.212390	-0.683592	7.804329	-0.235096	-0.690483	7.875041	-0.239816	-0.694144	7.837997
70	H	-1.899259	2.380302	-7.424311	-1.900250	2.377810	-7.525756	-1.893767	2.369506	-7.472905
71	H	-0.212758	0.683858	-7.804597	-0.235391	0.690706	-7.875268	-0.240148	0.694384	-7.838249
72	H	-1.163604	-3.687107	-8.014686	-1.175935	-3.720829	-8.083972	-1.164578	-3.708671	-8.045970
73	H	0.407126	-5.301192	-7.123123	0.389461	-5.342675	-7.249499	0.389096	-5.314804	-7.202424
74	H	0.407166	-7.123100	-5.301181	0.389494	-7.249486	-5.342664	0.389147	-7.202394	-5.314794
75	H	-1.163537	-8.014773	-3.687132	-1.175891	-8.084049	-3.720840	-1.164499	-8.046064	-3.708697
76	H	-0.212600	-7.804506	0.683771	-0.235220	-7.875174	0.690596	-0.239967	-7.838138	0.694270
77	H	-1.899132	-7.424520	2.380258	-1.900118	-7.525955	2.377748	-1.893628	-7.473111	2.369453
78	H	2.160596	-3.687041	8.014690	2.191179	-3.720779	8.083977	2.173597	-3.708629	8.045989
79	H	0.589857	-5.301151	7.123175	0.625778	-5.342638	7.249541	0.619924	-5.314775	7.202451
80	H	1.209475	7.804398	0.683670	1.250426	7.875132	0.690560	1.248980	7.838078	0.694248

81	H	2.896034	7.424551	2.380164	2.915339	7.525941	2.377714	2.902636	7.473094	2.369404
82	H	1.209596	-7.804537	-0.683783	1.250492	-7.875215	-0.690619	1.249027	-7.838177	-0.694287
83	H	2.896129	-7.424478	-2.380249	2.915385	-7.525902	-2.377755	2.902689	-7.473062	-2.369445
84	H	0.589808	-7.123099	5.301194	0.625739	-7.249483	5.342682	0.619875	-7.202383	5.314815
85	H	2.160530	-8.014744	3.687143	2.191137	-8.084023	3.720858	2.173537	-8.046037	3.708717
86	H	2.895929	-2.380108	-7.424707	2.915252	-2.377666	-7.526042	2.902556	-2.369374	-7.473216
87	H	1.209341	-0.683593	-7.804314	1.250336	-0.690517	-7.875053	1.248869	-0.694189	-7.838010
88	H	2.896272	2.380383	7.424250	2.915486	2.377853	7.525726	2.902793	2.369547	7.472886
89	H	1.209784	0.683953	7.804652	1.250638	0.690760	7.875287	1.249176	0.694427	7.838271
90	H	0.589746	7.123012	-5.301210	0.625697	7.249431	-5.342690	0.619857	7.202353	-5.314805
91	H	2.160440	8.014734	-3.687185	2.191086	8.084017	-3.720868	2.173503	8.046007	-3.708728
92	H	2.160395	3.687202	-8.014795	2.191025	3.720895	-8.084064	2.173456	3.708745	-8.046068
93	H	0.589714	5.301190	-7.122996	0.625664	5.342681	-7.249402	0.619822	5.314790	-7.202337
94	Tv	5.453969	0.000000	0.000000	5.553867	0.000000	0.000000	5.519925	0.000000	0.000000

	Atomic Type	SiNT [110] - LDA			SiNT [110] - GGA			SiNT [110] - HSE		
		x	y	z	x	y	z	x	y	z
1	Si	-0.963615	15.343987	-0.000448	-0.972435	15.536021	0.000838	-0.972516	15.451563	-0.000033
2	Si	-0.985511	8.167899	-11.140353	-1.051035	8.270489	-11.286093	-0.990871	8.228885	-11.228083
3	Si	-0.956922	9.888010	-7.001530	-1.006459	10.029417	-7.105999	-0.968762	9.975171	-7.068836
4	Si	-0.964350	7.912835	-5.735911	-1.005733	8.031050	-5.825569	-0.973975	7.986638	-5.795380
5	Si	-0.961100	11.728849	-5.558744	-1.000979	11.881424	-5.629059	-0.971406	11.819064	-5.601047
6	Si	-0.654057	6.312027	-12.520154	-0.749106	6.394081	-12.689945	-0.684164	6.362430	-12.625290
7	Si	-1.024021	4.340970	-11.326823	-1.083814	4.396215	-11.474442	-1.020856	4.374535	-11.416378
8	Si	-0.651889	2.473134	-12.676880	-0.748815	2.499319	-12.843537	-0.681845	2.489707	-12.781027
9	Si	-0.962667	13.496925	-1.438611	-0.979812	13.670234	-1.459416	-0.972010	13.594326	-1.452281
10	Si	-0.963689	9.663474	-1.616334	-0.982643	9.790126	-1.636094	-0.972702	9.734633	-1.628768
11	Si	-0.963518	7.696042	-0.340168	-0.976363	7.795903	-0.343502	-0.972331	7.750401	-0.343801
12	Si	-0.963585	11.519228	-0.177249	-0.974341	11.669796	-0.178858	-0.972419	11.603816	-0.178971
13	Si	-0.966170	6.069626	-7.191779	-1.015840	6.156105	-7.292387	-0.976067	6.122059	-7.254314
14	Si	-0.965640	4.094425	-5.924210	-1.008955	4.156565	-6.007854	-0.975205	4.132927	-5.976452
15	Si	-0.948337	2.248418	-7.365997	-1.002967	2.283280	-7.467959	-0.961041	2.270980	-7.429716
16	Si	-0.651989	-1.370554	-12.842615	-0.751115	-1.393990	-13.009764	-0.681989	-1.381868	-12.947653
17	Si	-1.008306	0.496397	-11.486893	-1.074074	0.497505	-11.629967	-1.008733	0.498399	-11.573355
18	Si	-0.965106	13.236746	3.929346	-0.953290	13.410517	3.976734	-0.972907	13.336428	3.956438
19	Si	-0.963583	9.423061	3.790002	-0.953874	9.555970	3.840691	-0.971705	9.500272	3.817724
20	Si	-0.965675	11.283761	5.219175	-0.947345	11.438006	5.287868	-0.973080	11.372091	5.258351
21	Si	-0.962547	7.436894	5.046415	-0.946722	7.560238	5.135282	-0.970590	7.514213	5.103885
22	Si	-0.963654	5.843260	-1.773573	-0.984862	5.943098	-1.825482	-0.972678	5.905084	-1.815429
23	Si	-0.948734	-1.603309	-7.531015	-1.005732	-1.635631	-7.634870	-0.961594	-1.622737	-7.596950
24	Si	-1.297489	0.267859	-6.171148	-1.323702	0.269290	-6.265584	-1.283504	0.269098	-6.230908
25	Si	-0.971156	9.174118	9.160034	-0.930784	9.307727	9.290590	-0.976298	9.254136	9.239631
26	Si	-0.654151	-5.207979	-13.016637	-0.755938	-5.287339	-13.188792	-0.684633	-5.253373	-13.125267
27	Si	-0.942692	7.235707	10.468411	-0.902538	7.343124	10.612578	-0.954739	7.297458	10.552100
28	Si	-1.024270	-3.347147	-11.657690	-1.088528	-3.400034	-11.807138	-1.021273	-3.376685	-11.749803
29	Si	-0.963590	5.578654	3.606364	-0.955602	5.682918	3.683259	-0.971518	5.646678	3.658287
30	Si	-0.961067	3.634183	4.918442	-0.947488	3.711469	5.001963	-0.968970	3.683352	4.967657
31	Si	-0.966731	-5.425978	-7.687490	-1.022778	-5.509682	-7.790490	-0.976610	-5.474981	-7.753458

32	Si	-0.965795	-3.566880	-6.254311	-1.013590	-3.626551	-6.340128	-0.975598	-3.602643	-6.309383
33	Si	-0.958848	5.372416	9.037975	-0.922653	5.455235	9.165947	-0.966399	5.420128	9.111795
34	Si	-0.906125	3.399456	10.311364	-0.875839	3.455835	10.455775	-0.926803	3.431628	10.395218
35	Si	-0.986013	-7.176127	-11.802539	-1.060257	-7.276271	-11.950191	-0.991552	-7.232932	-11.893717
36	Si	-0.977312	1.541709	8.876707	-0.939702	1.572916	9.005004	-0.981412	1.559729	8.950476
37	Si	-0.963523	-5.668607	-2.271100	-0.991291	-5.764744	-2.326026	-0.972746	-5.727055	-2.316682
38	Si	-0.957016	-9.247775	-7.828663	-1.017055	-9.385493	-7.936044	-0.968882	-9.330405	-7.900662
39	Si	-0.960833	-11.205895	-6.549901	-1.013192	-11.356913	-6.623128	-0.971190	-11.293797	-6.597415
40	Si	-0.964466	-7.388621	-6.397552	-1.014312	-7.503300	-6.489856	-0.974130	-7.458385	-6.461006
41	Si	-0.977628	-2.302584	8.711865	-0.942309	-2.335328	8.838485	-0.981857	-2.324230	8.783626
42	Si	-0.923140	-0.437958	10.140619	-0.891448	-0.438851	10.278322	-0.940204	-0.440161	10.218828
43	Si	-0.963502	-5.868173	3.111403	-0.962007	-5.975526	3.184703	-0.971620	-5.940444	3.158855
44	Si	-0.961224	-4.044980	4.587987	-0.952128	-4.124205	4.667806	-0.969372	-4.097335	4.633039
45	Si	-0.963467	-9.487988	-2.443930	-0.992924	-9.614124	-2.466280	-0.972547	-9.558738	-2.460634
46	Si	-0.962199	-13.322793	-2.597656	-0.993836	-13.495154	-2.621324	-0.971552	-13.419367	-2.616718
47	Si	-0.963220	-11.460859	-1.170507	-0.986507	-11.611009	-1.174784	-0.972095	-11.545446	-1.176993
48	Si	-0.963321	-7.637674	-1.002637	-0.984598	-7.737224	-1.008212	-0.972256	-7.692107	-1.009783
49	Si	-0.959460	-6.132654	8.541885	-0.929652	-6.217181	8.667573	-0.966985	-6.184160	8.612364
50	Si	-0.906444	-4.276538	9.981000	-0.880572	-4.334738	10.123347	-0.927251	-4.313007	10.062082
51	Si	-0.963386	-9.714707	2.962954	-0.964176	-9.847679	3.010523	-0.971570	-9.793230	2.985866
52	Si	-0.964652	-13.525888	2.772621	-0.967290	-13.699568	2.817065	-0.972462	-13.626879	2.794070
53	Si	-0.962604	-7.843653	4.385595	-0.955229	-7.969766	4.471163	-0.970698	-7.925184	4.438468
54	Si	-0.965377	-11.691371	4.226445	-0.959543	-11.846021	4.291950	-0.972831	-11.781685	4.260303
55	Si	-0.971289	-9.929656	8.334184	-0.941387	-10.065668	8.462239	-0.976462	-10.014419	8.409342
56	Si	-0.943124	-8.112029	9.806231	-0.911641	-8.221353	9.947851	-0.955317	-8.178116	9.885954
57	Si	-0.963057	-15.286817	-1.324297	-0.988201	-15.478546	-1.325714	-0.971904	-15.394423	-1.329655
58	Si	0.963055	15.286820	1.324290	0.988929	15.478550	1.325559	0.971900	15.394427	1.329643
59	Si	0.964652	13.525886	-2.772623	0.968027	13.699564	-2.817203	0.972460	13.626874	-2.794072
60	Si	0.971291	9.929653	-8.334184	0.942137	10.065654	-8.462419	0.976464	10.014413	-8.409344
61	Si	0.959458	6.132656	-8.541889	0.930434	6.217285	-8.667746	0.966983	6.184180	-8.612367
62	Si	0.943121	8.112030	-9.806237	0.912338	8.221403	-9.948113	0.955298	8.178124	-9.885975
63	Si	0.962199	13.322799	2.597653	0.994569	13.495176	2.621194	0.971549	13.419378	2.616717
64	Si	0.906443	4.276535	-9.980997	0.881515	4.334700	-10.123326	0.927269	4.312999	-10.062049
65	Si	0.963384	9.714710	-2.962958	0.964923	9.847738	-3.010664	0.971569	9.793242	-2.985866
66	Si	0.963505	5.868168	-3.111403	0.962809	5.975515	-3.184897	0.971635	5.940435	-3.158860
67	Si	0.962605	7.843651	-4.385592	0.956031	7.969805	-4.471270	0.970709	7.925187	-4.438456
68	Si	0.965374	11.691372	-4.226452	0.960270	11.846049	-4.292136	0.972823	11.781689	-4.260317
69	Si	0.977630	2.302580	-8.711864	0.943288	2.335169	-8.838669	0.981886	2.324203	-8.783621
70	Si	0.923136	0.437959	-10.140626	0.892130	0.438839	-10.278684	0.940175	0.440161	-10.218861
71	Si	0.906124	-3.399456	-10.311363	0.876756	-3.455857	-10.455770	0.926819	-3.431628	-10.395187
72	Si	0.961217	4.044980	-4.587993	0.952624	4.124238	-4.668062	0.969334	4.097338	-4.633061
73	Si	0.963467	9.487987	2.443928	0.993667	9.614088	2.466138	0.972547	9.558732	2.460634
74	Si	0.963222	11.460860	1.170509	0.987262	11.611004	1.174688	0.972098	11.545447	1.177003
75	Si	0.957018	9.247782	7.828662	1.017795	9.385505	7.935870	0.968882	9.330418	7.900661
76	Si	0.963525	5.668613	2.271099	0.992071	5.764783	2.325820	0.972758	5.727066	2.316676
77	Si	0.963314	7.637677	1.002631	0.985289	7.737241	1.007991	0.972239	7.692111	1.009768
78	Si	0.977313	-1.541705	-8.876709	0.940637	-1.572806	-9.005193	0.981435	-1.559707	-8.950473
79	Si	0.961061	-3.634181	-4.918450	0.947953	-3.711497	-5.002252	0.968932	-3.683353	-4.967682

80	Si	0.966731	5.425976	7.687486	1.023515	5.509582	7.790308	0.976611	5.474967	7.753453
81	Si	0.960830	11.205898	6.549895	1.013906	11.356914	6.622944	0.971182	11.293802	6.597401
82	Si	0.965788	3.566881	6.254304	1.014044	3.626550	6.339824	0.975561	3.602644	6.309356
83	Si	0.964467	7.388624	6.397556	1.015111	7.503261	6.489750	0.974140	7.458385	6.461020
84	Si	0.948735	1.603314	7.531013	1.006509	1.635738	7.634705	0.961619	1.622759	7.596953
85	Si	1.024269	3.347148	11.657692	1.089433	3.400046	11.807157	1.021290	3.376689	11.749835
86	Si	0.958847	-5.372419	-9.037979	0.923435	-5.455378	-9.166140	0.966400	-5.420152	-9.111799
87	Si	0.654151	5.207983	13.016635	0.756796	5.287404	13.188715	0.684635	5.253389	13.125277
88	Si	0.942690	-7.235709	-10.468419	0.903218	-7.343201	-10.612861	0.954719	-7.297468	-10.552124
89	Si	0.986011	7.176129	11.802532	1.060936	7.276234	11.949906	0.991532	7.232932	11.893694
90	Si	1.297489	-0.267859	6.171154	1.324551	-0.269310	6.265537	1.283524	-0.269100	6.230945
91	Si	0.965633	-4.094424	5.924204	1.009433	-4.156559	6.007573	0.975168	-4.132923	5.976427
92	Si	0.963614	-15.343987	0.000441	0.973163	-15.536017	-0.000994	0.972512	-15.451564	0.000021
93	Si	0.963591	-5.578648	-3.606365	0.956377	-5.682900	-3.683466	0.971530	-5.646668	-3.658293
94	Si	0.971158	-9.174114	-9.160035	0.931517	-9.307736	-9.290770	0.976298	-9.254131	-9.239633
95	Si	0.651989	1.370552	12.842614	0.751941	1.393888	13.009567	0.681988	1.381854	12.947651
96	Si	1.008303	-0.496396	11.486886	1.074774	-0.497506	11.629596	1.008703	-0.498396	11.573321
97	Si	0.948339	-2.248422	7.365997	1.003796	-2.283405	7.467811	0.961073	-2.271001	7.429722
98	Si	1.024020	-4.340971	11.326826	1.084744	-4.396268	11.474474	1.020875	-4.374542	11.416412
99	Si	0.963582	-9.423063	-3.790004	0.954617	-9.556037	-3.840830	0.971704	-9.500284	-3.817723
100	Si	0.962548	-7.436891	-5.046412	0.947511	-7.560294	-5.135392	0.970600	-7.514217	-5.103873
101	Si	0.963656	-5.843264	1.773573	0.985666	-5.943116	1.825285	0.972692	-5.905092	1.815423
102	Si	0.963510	-7.696042	0.340162	0.977057	-7.795894	0.343282	0.972314	-7.750400	0.343786
103	Si	0.651888	-2.473132	12.676877	0.749645	-2.499234	12.843353	0.681844	-2.489691	12.781025
104	Si	0.965105	-13.236742	-3.929349	0.954021	-13.410517	-3.976869	0.972904	-13.336422	-3.956441
105	Si	0.966168	-6.069623	7.191775	1.016577	-6.156014	7.292223	0.976065	-6.122043	7.254310
106	Si	0.963687	-9.663472	1.616331	0.983387	-9.790080	1.635947	0.972700	-9.734624	1.628766
107	Si	0.965673	-11.283759	-5.219182	0.948062	-11.438037	-5.288053	0.973072	-11.372093	-5.258365
108	Si	0.956924	-9.888017	7.001530	1.007216	-10.029425	7.105822	0.968763	-9.975181	7.068834
109	Si	0.964351	-7.912838	5.735914	1.006545	-8.031013	5.825466	0.973986	-7.986637	5.795393
110	Si	0.963587	-11.519230	0.177251	0.975097	-11.669790	0.178761	0.972422	-11.603816	0.178981
111	Si	0.962667	-13.496929	1.438609	0.980550	-13.670250	1.459284	0.972009	-13.594335	1.452279
112	Si	0.654057	-6.312030	12.520154	0.749985	-6.394179	12.689874	0.684167	-6.362447	12.625301
113	Si	0.985509	-8.167898	11.140347	1.051732	-8.270469	11.285827	0.990852	-8.228883	11.228063
114	Si	0.961096	-11.728850	5.558737	1.001704	-11.881418	5.628872	0.971398	-11.819064	5.601034
115	H	-0.963743	16.595706	-0.846768	-0.976535	16.792722	-0.835546	-0.972762	16.698295	-0.830753
116	H	-0.963191	-16.460984	-2.275264	-0.993546	-16.659307	-2.266245	-0.972107	-16.565144	-2.264431
117	H	0.963190	16.460988	2.275255	0.994277	16.659314	2.266078	0.972103	16.565152	2.264416
118	H	0.963742	-16.595708	0.846758	0.977267	-16.792720	0.835377	0.972758	-16.698298	0.830737
119	H	-0.963799	4.585334	-0.933288	-0.981171	4.668448	-1.016964	-0.972643	4.640802	-1.011792
120	H	0.963531	4.487134	1.326318	0.986904	4.564226	1.410932	0.972666	4.536925	1.406879
121	H	0.960831	2.758263	-3.791657	0.956233	2.854676	-3.850723	0.969240	2.836338	-3.823399
122	H	-0.737519	0.208561	-4.775242	-0.730301	0.209872	-4.887650	-0.686575	0.210302	-4.867402
123	H	-0.960465	2.422152	4.012456	-0.952139	2.517244	4.077950	-0.968567	2.497432	4.051522
124	H	-0.960836	-2.758266	3.791647	-0.955697	-2.854617	3.850481	-0.969261	-2.836339	3.823374
125	H	0.737524	-0.208564	4.775247	0.731200	-0.209914	4.887585	0.686605	-0.210310	4.867435
126	H	0.963801	-4.585334	0.933293	0.981957	-4.668433	1.016807	0.972656	-4.640802	1.011799
127	H	-0.963530	-4.487133	-1.326315	-0.986137	-4.564219	-1.411104	-0.972655	-4.536923	-1.406873

128	H	0.960462	-2.422147	-4.012467	0.952630	-2.517270	-4.078263	0.968547	-2.497429	-4.051550
129	H	0.965088	-14.427383	-4.861149	0.948854	-14.604364	-4.901594	0.972770	-14.520757	-4.874673
130	H	-0.961182	-12.396218	-7.481790	-1.018552	-12.552344	-7.545738	-0.971534	-12.479608	-7.513652
131	H	0.968406	-10.378666	-10.073783	0.924488	-10.506605	-10.208997	0.974323	-10.443375	-10.151530
132	H	-0.970239	-8.380396	-12.714614	-1.053638	-8.473749	-12.869115	-0.980023	-8.421939	-12.804761
133	H	-0.969652	9.446389	-11.945079	-1.043348	9.541854	-12.099687	-0.979384	9.491684	-12.033734
134	H	0.968577	11.208998	-9.139923	0.936388	11.338788	-9.274556	0.974443	11.277945	-9.215189
135	H	-0.961423	12.995122	-6.384481	-1.005070	13.151548	-6.445790	-0.971794	13.079548	-6.411508
136	H	0.964651	14.792312	-3.598507	0.964134	14.967968	-3.636688	0.972282	14.885796	-3.607061
137	H	-0.965087	14.427384	4.861150	-0.948109	14.604316	4.901502	-0.972771	14.520753	4.874683
138	H	0.961180	12.396223	7.481782	1.019276	12.552341	7.545526	0.971529	12.479615	7.513635
139	H	-0.968405	10.378663	10.073790	-0.923719	10.506533	10.208862	-0.974317	10.443364	10.151548
140	H	0.970237	8.380400	12.714605	1.054360	8.473753	12.868747	0.980010	8.421948	12.804730
141	H	0.969649	-9.446390	11.945071	1.044078	-9.541866	12.099337	0.979371	-9.491689	12.033705
142	H	-0.968575	-11.208997	9.139930	-0.935605	-11.338757	9.274403	-0.974435	-11.277940	9.215204
143	H	0.961420	-12.995125	6.384471	1.005805	-13.151533	6.445578	0.971788	-13.079551	6.411492
144	H	-0.964650	-14.792312	3.598510	-0.963383	-14.967930	3.636587	-0.972282	-14.885792	3.607071
145	H	-0.850525	5.169296	13.195511	-0.727910	5.254221	13.429696	-0.786986	5.219295	13.365137
146	H	1.204191	1.304862	14.239461	1.346873	1.327031	14.386384	1.280017	1.316082	14.310177
147	H	-0.855110	-2.486128	12.846567	-0.738026	-2.511886	13.073030	-0.792230	-2.503782	13.011734
148	H	1.215831	-6.374990	13.912507	1.356196	-6.463007	14.061043	1.291714	-6.429424	13.982952
149	H	-1.215827	6.374981	-13.912508	-1.355314	6.462644	-14.061145	-1.291707	6.429363	-13.982941
150	H	-1.203721	2.526375	-14.074411	-1.343588	2.551140	-14.221086	-1.279775	2.541178	-14.144222
151	H	-1.204188	-1.304869	-14.239463	-1.346091	-1.327412	-14.386583	-1.280016	-1.316145	-14.310179
152	H	-1.215105	-5.150807	-14.409594	-1.362015	-5.237495	-14.560868	-1.292134	-5.203144	-14.483671
153	H	1.215107	5.150814	14.409591	1.362878	5.237829	14.560782	1.292139	5.203202	14.483684
154	H	-0.854944	1.370191	13.013235	-0.735680	1.390045	13.239797	-0.792066	1.377383	13.178839
155	H	1.203723	-2.526367	14.074408	1.344367	-2.550777	14.220928	1.279773	-2.541113	14.144224
156	H	-0.850432	-6.288139	12.702626	-0.734660	-6.379102	12.932895	-0.787456	-6.348279	12.867109
157	H	0.850432	6.288134	-12.702623	0.735560	6.379167	-12.932931	0.787458	6.348282	-12.867094
158	H	0.855109	2.486131	-12.846568	0.738847	2.511896	-13.073252	0.792225	2.503779	-13.011737
159	H	0.854943	-1.370192	-13.013234	0.736499	-1.390087	-13.240026	0.792062	-1.377380	-13.178839
160	H	0.850524	-5.169291	-13.195510	0.728790	-5.254321	-13.429748	0.786986	-5.219300	-13.365126
161	H	2.803677	-0.261278	5.991209	2.813167	-0.261559	6.037693	2.758504	-0.260123	6.001694
162	H	-2.803676	0.261277	-5.991199	-2.812155	0.261511	-6.037233	-2.758484	0.260124	-6.001659
163	Tv	3.853944	-0.000161	0.000603	3.909231	-0.001159	-0.020036	3.888840	-0.000017	-0.000208

	Atomic Type	SiNW [110] - LDA			SiNW [110] - GGA			SiNW [110] - HSE		
		x	y	z	x	y	z	x	y	z
1	Si	-0.939601	15.350424	0.001407	-0.965993	15.535464	-0.014540	-0.959582	15.453578	-0.012204
2	Si	-0.910615	8.172374	-11.153182	-0.900463	8.257484	-11.293850	-0.890829	8.217197	-11.233765
3	Si	-0.941742	9.906653	-7.018821	-0.940915	10.018159	-7.113563	-0.931880	9.966634	-7.074517
4	Si	-0.935122	7.930959	-5.753995	-0.941602	8.020531	-5.830918	-0.933638	7.979032	-5.798741
5	Si	-0.937869	11.740359	-5.564682	-0.943704	11.873606	-5.642197	-0.935340	11.813924	-5.611825
6	Si	-1.245254	6.312336	-12.526207	-1.208760	6.378708	-12.691387	-1.195083	6.348088	-12.626257
7	Si	-0.879114	4.341829	-11.330397	-0.875396	4.382631	-11.472564	-0.867162	4.361964	-11.412055
8	Si	-1.242414	2.475728	-12.684448	-1.207106	2.490961	-12.847230	-1.194842	2.481563	-12.783486
9	Si	-0.939559	13.504230	-1.437906	-0.960691	13.668511	-1.473126	-0.953681	13.595042	-1.462657

10	Si	-0.937877	9.668267	-1.614858	-0.959700	9.785247	-1.645190	-0.953183	9.732719	-1.635110
11	Si	-0.937947	7.693282	-0.344324	-0.965216	7.787154	-0.357247	-0.959228	7.745127	-0.354284
12	Si	-0.939429	11.525660	-0.176917	-0.966052	11.668190	-0.192484	-0.959804	11.604709	-0.189221
13	Si	-0.932253	6.077937	-7.198591	-0.933658	6.143738	-7.292029	-0.925944	6.112340	-7.252108
14	Si	-0.931492	4.100713	-5.927779	-0.938919	4.143859	-6.003046	-0.931183	4.122980	-5.970416
15	Si	-0.933565	2.240989	-7.364192	-0.934781	2.260428	-7.455951	-0.926329	2.250471	-7.416485
16	Si	-1.242088	-1.367165	-12.851443	-1.207049	-1.398495	-13.011697	-1.194917	-1.386473	-12.948027
17	Si	-0.880369	0.499122	-11.497380	-0.876004	0.491524	-11.634662	-0.867399	0.492650	-11.574905
18	Si	-0.940857	13.245698	3.935606	-0.983044	13.409710	3.965616	-0.978503	13.338503	3.948791
19	Si	-0.942313	9.434006	3.793638	-0.984346	9.553569	3.825744	-0.979578	9.500836	3.807257
20	Si	-0.940757	11.292833	5.225380	-0.988486	11.435414	5.273406	-0.984434	11.372704	5.248041
21	Si	-0.943949	7.458981	5.065468	-0.991072	7.555950	5.116137	-0.987051	7.513485	5.090097
22	Si	-0.937097	5.835767	-1.783027	-0.959132	5.905178	-1.811731	-0.952571	5.873813	-1.801573
23	Si	-0.937592	3.860583	-0.511352	-0.965028	3.907119	-0.522035	-0.959345	3.886228	-0.519232
24	Si	-0.935359	2.004430	-1.952151	-0.958044	2.026681	-1.978842	-0.952064	2.016376	-1.968710
25	Si	-0.933190	-1.594917	-7.531042	-0.934493	-1.623611	-7.620386	-0.926162	-1.612212	-7.581227
26	Si	-0.930796	0.264304	-6.093355	-0.938645	0.260512	-6.167230	-0.931216	0.261116	-6.135073
27	Si	-0.937158	9.181973	9.182215	-1.002234	9.303547	9.276797	-1.000378	9.252740	9.230780
28	Si	-1.244175	-5.203171	-13.026532	-1.207616	-5.285576	-13.185131	-1.195407	-5.252474	-13.120806
29	Si	-0.966113	7.236098	10.481130	-1.030412	7.338403	10.596489	-1.028911	7.295150	10.540655
30	Si	-0.878426	-3.343606	-11.664372	-0.875191	-3.399483	-11.801799	-0.867684	-3.376868	-11.741768
31	Si	-0.939344	5.601378	3.628430	-0.982611	5.673938	3.663895	-0.978544	5.642208	3.644669
32	Si	-0.940549	3.628569	4.903832	-0.988882	3.678627	4.957830	-0.985389	3.657165	4.930977
33	Si	-0.941610	1.769691	3.465328	-0.984175	1.795229	3.503790	-0.980215	1.784619	3.483975
34	Si	-0.935308	-1.828185	-2.118546	-0.958153	-1.852746	-2.142802	-0.952365	-1.841765	-2.132985
35	Si	-0.937031	0.029385	-0.678696	-0.964749	0.029040	-0.686987	-0.959446	0.029230	-0.684330
36	Si	-0.930927	-5.431701	-7.698616	-0.933086	-5.506807	-7.784669	-0.926251	-5.473957	-7.745463
37	Si	-0.930901	-3.571741	-6.261163	-0.938747	-3.622570	-6.331489	-0.931583	-3.600468	-6.299338
38	Si	-0.958331	5.375367	9.045974	-1.018373	5.452720	9.146218	-1.015480	5.419808	9.097354
39	Si	-0.947841	3.396455	10.310179	-1.015225	3.451652	10.429942	-1.012699	3.429246	10.374141
40	Si	-0.908832	-7.175325	-11.820255	-0.899401	-7.275449	-11.950941	-0.891171	-7.233008	-11.891972
41	Si	-0.925887	1.536980	8.874517	-0.994218	1.567248	8.978082	-0.992486	1.555698	8.929038
42	Si	-0.939920	-2.064098	3.298400	-0.983309	-2.084977	3.339247	-0.979661	-2.074552	3.319213
43	Si	-0.940821	-0.206112	4.736860	-0.989169	-0.203045	4.794175	-0.985911	-0.203207	4.766846
44	Si	-0.935991	-5.659793	-2.283017	-0.958863	-5.731565	-2.304304	-0.953196	-5.699611	-2.294976
45	Si	-0.936916	-3.802209	-0.844573	-0.964950	-3.849425	-0.850334	-0.959738	-3.828091	-0.848176
46	Si	-0.939832	-9.261941	-7.852103	-0.940166	-9.382756	-7.934471	-0.932303	-9.329672	-7.896961
47	Si	-0.936183	-11.214404	-6.562313	-0.943448	-11.355504	-6.625020	-0.936834	-11.294312	-6.596549
48	Si	-0.933662	-7.403001	-6.420684	-0.941171	-7.500263	-6.487728	-0.934391	-7.457576	-6.456691
49	Si	-0.955298	-2.300344	8.710005	-1.017072	-2.319238	8.815886	-1.015254	-2.308921	8.766213
50	Si	-0.945658	-0.439217	10.144006	-1.014731	-0.432681	10.264580	-1.013196	-0.433567	10.208886
51	Si	-0.941509	-5.894803	3.129403	-0.984716	-5.962826	3.172096	-0.981279	-5.931207	3.151925
52	Si	-0.945086	-4.039759	4.571318	-0.992540	-4.083579	4.629966	-0.989678	-4.062598	4.602601
53	Si	-0.936765	-9.492161	-2.447426	-0.959702	-9.611677	-2.465737	-0.954628	-9.558458	-2.457041
54	Si	-0.937146	-13.329159	-2.604021	-0.960211	-13.495633	-2.622295	-0.955217	-13.421510	-2.613863
55	Si	-0.937259	-11.467040	-1.176178	-0.965523	-11.610327	-1.177296	-0.961067	-11.546445	-1.175735
56	Si	-0.937621	-7.634421	-1.010376	-0.965612	-7.729149	-1.013657	-0.960764	-7.686746	-1.011755
57	Si	-0.946608	-6.138733	8.547345	-1.010570	-6.204523	8.654284	-1.008621	-6.172863	8.604637

58	Si	-0.993496	-4.277027	9.979532	-1.052072	-4.319398	10.103831	-1.050616	-4.298402	10.047370
59	Si	-0.939687	-9.727076	2.961011	-0.983304	-9.842096	3.005226	-0.980249	-9.789673	2.985330
60	Si	-0.938630	-13.536961	2.771238	-0.982662	-13.696378	2.818637	-0.979967	-13.625521	2.799543
61	Si	-0.941164	-7.869643	4.399912	-0.989821	-7.960450	4.460175	-0.987101	-7.918401	4.432847
62	Si	-0.938485	-11.703085	4.225576	-0.987782	-11.839350	4.288534	-0.985573	-11.777195	4.261382
63	Si	-0.935561	-9.943986	8.350215	-1.002211	-10.053630	8.457447	-1.001003	-10.004085	8.409703
64	Si	-0.964343	-8.118148	9.813248	-1.028958	-8.206777	9.938338	-1.028440	-8.165075	9.881488
65	Si	-0.937012	-15.293094	-1.330580	-0.965687	-15.478926	-1.326803	-0.961396	-15.396540	-1.326964
66	Si	0.983698	15.292995	1.329189	0.978569	15.478565	1.331431	0.974150	15.396348	1.329565
67	Si	0.985199	13.537636	-2.773165	0.995494	13.696732	-2.814456	0.992760	13.625878	-2.797295
68	Si	0.982053	9.945171	-8.352497	1.014430	10.054509	-8.453412	1.013685	10.004797	-8.407699
69	Si	0.993542	6.140367	-8.549455	1.023487	6.205776	-8.650845	1.021344	6.173836	-8.602664
70	Si	1.010748	8.119567	-9.815828	1.042102	8.208150	-9.934861	1.041308	8.165923	-9.879688
71	Si	0.983869	13.328824	2.602298	0.973127	13.494994	2.626524	0.967936	13.421142	2.616215
72	Si	1.039738	4.278568	-9.981113	1.064719	4.320295	-10.099555	1.062567	4.299366	-10.044974
73	Si	0.986997	9.727890	-2.963585	0.996639	9.842360	-3.001763	0.993387	9.790059	-2.983592
74	Si	0.987887	5.895063	-3.132353	0.997314	5.962718	-3.168938	0.994139	5.931232	-3.150592
75	Si	0.988117	7.870332	-4.402261	1.002813	7.960648	-4.456598	0.999970	7.918769	-4.431040
76	Si	0.985688	11.704037	-4.227923	1.001055	11.839892	-4.284627	0.998586	11.777740	-4.259419
77	Si	0.991635	2.300810	-8.713385	1.021848	2.319342	-8.812980	1.020482	2.309124	-8.765301
78	Si	1.038808	0.440387	-10.148115	1.064397	0.433515	-10.262514	1.062578	0.434401	-10.208490
79	Si	1.040504	-3.397855	-10.314769	1.064991	-3.453235	-10.428459	1.061942	-3.430729	-10.374393
80	Si	0.991347	4.040187	-4.574720	1.005140	4.083749	-4.627396	1.002024	4.062744	-4.601604
81	Si	0.982823	9.492147	2.444815	0.972202	9.611327	2.469156	0.967175	9.558218	2.458747
82	Si	0.989867	2.064038	-3.302563	0.998606	2.084743	-3.337295	0.994832	2.074281	-3.318861
83	Si	0.983734	11.467147	1.173897	0.978311	11.610082	1.181010	0.973750	11.546342	1.177728
84	Si	0.985470	3.801997	0.840930	0.979226	3.848947	0.852907	0.974077	3.827821	0.848967
85	Si	0.986577	9.260420	7.849909	0.953107	9.381152	7.938374	0.945194	9.328438	7.898923
86	Si	0.985417	5.659840	2.279156	0.973670	5.731269	2.306767	0.967985	5.699455	2.295706
87	Si	0.985287	7.634777	1.007205	0.979182	7.729075	1.016653	0.974357	7.686813	1.012987
88	Si	0.992077	0.205742	-4.740912	1.005450	0.202364	-4.791939	1.002077	0.202729	-4.766501
89	Si	0.992017	-1.537073	-8.880290	1.022146	-1.567676	-8.977526	1.020647	-1.556106	-8.930182
90	Si	0.991912	-3.628420	-4.907973	1.005278	-3.678865	-4.955713	1.001594	-3.657153	-4.930404
91	Si	0.969350	5.431203	7.695052	0.940384	5.506085	7.787236	0.933396	5.473483	7.746662
92	Si	0.982812	11.213315	6.560580	0.956260	11.354231	6.629239	0.949476	11.293390	6.598839
93	Si	0.983631	1.828035	2.114941	0.972466	1.852275	2.145343	0.966674	1.841574	2.133856
94	Si	0.985836	-0.029277	0.674771	0.979351	-0.029191	0.689124	0.973851	-0.029255	0.684991
95	Si	0.989952	-1.769867	-3.469003	0.998526	-1.795753	-3.501290	0.994547	-1.784794	-3.483146
96	Si	0.982768	3.571857	6.256870	0.955592	3.622352	6.333455	0.948249	3.600600	6.299816
97	Si	0.986176	-3.860813	0.507706	0.979306	-3.907604	0.524603	0.973691	-3.886552	0.520017
98	Si	0.978728	7.402403	6.417371	0.952875	7.499488	6.490598	0.946136	7.456889	6.457932
99	Si	0.995837	1.594790	7.525922	0.959391	1.623153	7.621551	0.951405	1.611865	7.580652
100	Si	0.974380	3.342413	11.660029	0.928432	3.397791	11.803490	0.920334	3.375424	11.741725
101	Si	0.994895	-5.376186	-9.049783	1.024115	-5.453706	-9.143850	1.021140	-5.420477	-9.096294
102	Si	1.303781	5.205311	13.028734	1.230958	5.285974	13.192008	1.217624	5.253321	13.125757
103	Si	1.012501	-7.238368	-10.483178	1.043079	-7.340711	-10.592473	1.040728	-7.296896	-10.538305
104	Si	0.955827	7.173179	11.818678	0.912538	7.273030	11.955365	0.903518	7.231203	11.894712
105	Si	0.982534	-0.264796	6.089143	0.955371	-0.261379	6.169319	0.947795	-0.261720	6.135232

106	Si	0.985109	-2.004450	1.948043	0.973178	-2.026903	1.980876	0.967062	-2.016555	1.969147
107	Si	0.977228	-4.100207	5.924394	0.951088	-4.143522	6.005617	0.943115	-4.122752	5.971421
108	Si	0.986284	-15.350270	-0.002822	0.978870	-15.535582	0.019157	0.972338	-15.453601	0.014792
109	Si	0.988991	-5.601312	-3.632364	0.997604	-5.674213	-3.661506	0.993552	-5.642295	-3.644005
110	Si	0.983999	-9.184060	-9.184252	1.015231	-9.305647	-9.272750	1.013303	-9.254467	-9.228674
111	Si	0.636895	1.366539	12.857706	0.607812	1.397971	13.019754	0.602134	1.386429	12.953993
112	Si	0.976683	-0.497921	11.493651	0.928927	-0.490672	11.637040	0.919721	-0.491590	11.575498
113	Si	0.971746	-2.240835	7.360900	0.941138	-2.260705	7.458911	0.933142	-2.250501	7.417515
114	Si	0.926099	-4.340214	11.329220	0.888674	-4.381691	11.477223	0.879382	-4.360697	11.414809
115	Si	0.988195	-9.434139	-3.796265	0.996708	-9.554025	-3.822342	0.991991	-9.501196	-3.805546
116	Si	0.989548	-7.459384	-5.068751	1.003203	-7.556587	-5.113238	0.999176	-7.514012	-5.088828
117	Si	0.983710	-5.835570	1.780053	0.971953	-5.905331	1.814835	0.965625	-5.873820	1.802862
118	Si	0.985447	-7.692860	0.341209	0.978649	-7.787174	0.360306	0.972677	-7.745044	0.355571
119	Si	1.302613	-2.478687	12.686222	1.230179	-2.492924	12.854001	1.216336	-2.483370	12.788547
120	Si	0.987597	-13.246232	-3.937274	0.995971	-13.410534	-3.961336	0.991215	-13.339034	-3.946403
121	Si	0.979088	-6.076751	7.196183	0.946560	-6.142957	7.295233	0.938686	-6.111584	7.253847
122	Si	0.985221	-9.667621	1.612186	0.973059	-9.785092	1.648593	0.966354	-9.732427	1.636778
123	Si	0.987332	-11.293547	-5.227223	1.001272	-11.436397	-5.269286	0.997088	-11.373403	-5.245841
124	Si	0.988277	-9.905833	7.016581	0.953169	-10.017627	7.117614	0.944591	-9.966103	7.076546
125	Si	0.982108	-7.930110	5.751798	0.954590	-8.020257	5.834622	0.946474	-7.978590	5.800686
126	Si	0.985968	-11.525354	0.174670	0.978888	-11.668271	0.196211	0.972541	-11.604666	0.191218
127	Si	0.986122	-13.503725	1.436005	0.973524	-13.668314	1.477313	0.966458	-13.594833	1.464922
128	Si	1.290494	-6.311759	12.523945	1.220630	-6.378316	12.695620	1.207120	-6.347391	12.628191
129	Si	0.957082	-8.171627	11.150461	0.913752	-8.256668	11.297277	0.903663	-8.216476	11.235552
130	Si	0.985045	-11.739400	5.562323	0.956977	-11.872964	5.646116	0.948347	-11.813306	5.613778
131	H	-0.938743	16.603176	-0.843396	-0.961811	16.791702	-0.851602	-0.955024	16.699797	-0.843646
132	H	-0.935899	-16.467910	-2.280754	-0.961462	-16.659967	-2.266983	-0.957005	-16.567522	-2.261386
133	H	0.982590	16.467671	2.279530	0.974344	16.659426	2.271827	0.969775	16.567220	2.264119
134	H	0.985426	-16.602823	0.842279	0.974687	-16.791680	0.856433	0.967768	-16.699688	0.846441
135	H	0.988548	-14.440040	-4.864975	1.000030	-14.603048	-4.887766	0.995451	-14.522554	-4.865661
136	H	-0.934963	-12.409038	-7.488835	-0.939206	-12.549831	-7.549021	-0.932431	-12.479257	-7.513881
137	H	0.987662	-10.382328	-10.106252	1.021019	-10.504422	-10.191122	1.018832	-10.443491	-10.140857
138	H	-0.923575	-8.376323	-12.736712	-0.907159	-8.473496	-12.869103	-0.898553	-8.422760	-12.802074
139	H	-2.749761	-5.167361	-13.201586	-2.693524	-5.253250	-13.420176	-2.666997	-5.219703	-13.362137
140	H	-2.749350	-1.360671	-13.019932	-2.695438	-1.389297	-13.237278	-2.668446	-1.376146	-13.182299
141	H	-2.749697	2.482540	-12.852862	-2.695493	2.499491	-13.072882	-2.668383	2.490500	-13.017635
142	H	-2.750546	6.290556	-12.705120	-2.695012	6.364975	-12.926726	-2.666552	6.335137	-12.870029
143	H	-0.925665	9.448397	-11.961928	-0.908048	9.528631	-12.107768	-0.898287	9.479597	-12.040061
144	H	0.985457	11.218980	-9.167003	1.020252	11.326711	-9.267019	1.019664	11.267230	-9.215247
145	H	-0.936824	13.010577	-6.384559	-0.939445	13.141625	-6.462134	-0.930683	13.072445	-6.425270
146	H	0.985813	14.807223	-3.594151	0.999459	14.963138	-3.636990	0.997134	14.883206	-3.612696
147	H	-0.941839	14.439489	4.863322	-0.987115	14.602212	4.892052	-0.982733	14.521959	4.868126
148	H	0.981452	12.407825	7.487255	0.951932	12.548503	7.553293	0.945021	12.478238	7.516284
149	H	-0.940786	10.380174	10.104298	-1.008112	10.502272	10.195211	-1.006081	10.441689	10.143063
150	H	0.967606	8.375439	12.733622	0.918224	8.471910	12.872492	0.909560	8.421599	12.804038
151	H	1.190378	1.306953	14.253939	1.191496	1.338692	14.401390	1.195738	1.327239	14.318372
152	H	0.750671	-2.528611	14.083637	0.637979	-2.541767	14.232589	0.612662	-2.531534	14.149111
153	H	2.795832	-6.289733	12.702802	2.706584	-6.364162	12.931662	2.678621	-6.333807	12.871967



154	H	0.972395	-9.447895	11.958808	0.921269	-9.528330	12.110362	0.911125	-9.479068	12.041557
155	H	-0.938792	-11.217480	9.165216	-1.007649	-11.325619	9.271371	-1.006921	-11.266431	9.217404
156	H	0.983990	-13.009721	6.382038	0.952704	-13.141111	6.465855	0.943737	-13.071905	6.427125
157	H	-0.939323	-14.806431	3.592402	-0.986676	-14.962761	3.641208	-0.984387	-14.882771	3.615075
158	H	0.743981	5.131344	14.421227	0.629870	5.220731	14.565504	0.606737	5.186374	14.481829
159	H	-0.687796	6.369139	-13.920596	-0.610568	6.439345	-14.066514	2.688582	5.236530	13.372059
160	H	-0.692820	2.535520	-14.082523	-0.617113	2.548198	-14.226581	-0.872236	1.377049	13.181769
161	H	-0.692402	-1.306479	-14.249433	-0.617109	-1.338841	-14.390969	2.688994	-2.508389	13.026142
162	H	-0.687935	-5.139073	-14.421104	-0.608243	-5.229296	-14.559887	0.599113	-6.407116	13.986069
163	H	2.808978	5.188563	13.209526	2.716659	5.268958	13.430011	-0.587096	6.407169	-13.984146
164	H	-0.869944	1.358338	13.031533	-0.881334	1.388727	13.239573	-0.594288	2.538826	-14.145214
165	H	2.809606	-2.504979	12.856781	2.718005	-2.516565	13.082058	-0.594425	-1.328112	-14.309753
166	H	0.733207	-6.368623	13.918395	0.621866	-6.439331	14.070528	-0.587648	-5.195698	-14.478900
167	Tv	3.848105	0.000343	0.002608	3.900755	-0.000674	0.017272	-0.890829	8.217197	-11.233765

	Atomic Type	SINT [111] - LDA			SINT [111] - GGA			SINT [111] - HSE		
		x	y	z	x	y	z	x	y	Z
1	Si	-4.633396	7.749789	0.000000	-4.753846	7.855040	0.000274	-4.721688	7.808117	0.000000
2	Si	-4.696863	6.094933	-3.529406	-4.830040	6.169981	-3.581107	-4.798561	6.141922	-3.563840
3	Si	-4.643364	3.894261	6.671509	-4.754146	3.959773	6.780363	-4.722622	3.934101	6.741096
4	Si	-4.622894	3.837411	-6.704735	-4.753014	3.892788	-6.820021	-4.720401	3.871792	-6.778358
5	Si	-4.584566	6.045856	3.463162	-4.701201	6.080716	3.489005	-4.667584	6.051535	3.473453
6	Si	-4.568443	-0.014756	-6.963170	-4.702092	-0.017784	-7.006729	-4.667443	-0.016531	-6.974562
7	Si	-4.713093	0.014945	7.042818	-4.828926	0.018130	7.133371	-4.798653	0.016825	7.099749
8	Si	-4.622938	-3.865778	-6.688311	-4.753071	-3.927351	-6.800627	-4.720421	-3.903874	-6.760019
9	Si	-4.643408	-3.865939	6.688054	-4.754209	-3.925214	6.800082	-4.722641	-3.902092	6.759611
10	Si	-4.696881	-6.109884	-3.503513	-4.829940	-6.188236	-3.550224	-4.798543	-6.158791	-3.534791
11	Si	-4.584573	-6.030991	3.488752	-4.701080	-6.062663	3.519380	-4.667559	-6.034928	3.501993
12	Si	-4.633401	-7.749737	0.032906	-4.753755	-7.854873	0.039746	-4.721666	-7.808026	0.036928
13	Si	-2.313545	3.865725	6.687962	-2.396535	3.927360	6.800400	-2.377143	3.903854	6.759815
14	Si	-2.239388	6.109982	3.503288	-2.319549	6.188328	3.550069	-2.298912	6.158848	3.534653
15	Si	-2.351687	6.030723	-3.489098	-2.448402	6.062514	-3.519586	-2.429892	6.034773	-3.502186
16	Si	-2.368138	0.014745	6.963293	-2.447568	0.017820	7.006796	-2.430171	0.016537	6.974622
17	Si	-2.302764	7.749615	-0.033314	-2.395687	7.854826	-0.040007	-2.375748	7.807954	-0.037166
18	Si	-2.293050	3.865930	-6.688593	-2.395377	3.925244	-6.800423	-2.374904	3.902095	-6.759926
19	Si	-2.313585	-3.837362	6.704390	-2.396591	-3.892724	6.819780	-2.377161	-3.871760	6.778136
20	Si	-2.239406	-6.095007	3.529181	-2.319446	-6.170017	3.580950	-2.298892	-6.141977	3.563695
21	Si	-2.351697	-6.045571	-3.463518	-2.448285	-6.080515	-3.489212	-2.429869	-6.051381	-3.473641
22	Si	-2.302768	-7.749650	-0.000415	-2.395597	-7.854943	-0.000539	-2.375725	-7.808055	-0.000241
23	Si	-2.293097	-3.894249	-6.672056	-2.395443	-3.959732	-6.780694	-2.374925	-3.934090	-6.741397
24	Si	-2.223474	-0.014949	-7.042909	-2.320725	-0.018096	-7.133429	-2.298954	-0.016822	-7.099802
25	Si	-1.527152	1.999743	7.876884	-1.616967	2.017108	7.974608	-1.602829	2.006397	7.935185
26	Si	-1.514302	7.827513	-2.243365	-1.615890	7.905957	-2.281730	-1.601253	7.867146	-2.268367
27	Si	-1.689720	4.091111	-2.373000	-1.669919	4.134197	-2.400801	-1.668387	4.111872	-2.386703
28	Si	-1.509576	5.828578	-5.664562	-1.617587	5.898648	-5.734576	-1.602230	5.869871	-5.705387
29	Si	-1.533651	5.966691	1.277825	-1.528520	6.111867	1.316608	-1.521137	6.066913	1.309911
30	Si	-1.520863	1.839184	-5.802237	-1.527374	1.883039	-5.960193	-1.519600	1.868988	-5.916841
31	Si	-1.539412	4.107684	4.489659	-1.528071	4.221715	4.611863	-1.521389	4.191289	4.577762

32	Si	-1.527171	-1.966340	7.885359	-1.617000	-1.976658	7.984516	-1.602835	-1.968781	7.944549
33	Si	-1.709555	0.010016	4.724611	-1.670144	0.012173	4.777587	-1.669626	0.011270	4.751699
34	Si	-1.533657	-5.961173	1.303134	-1.528424	-6.105075	1.347131	-1.521115	-6.060633	1.338543
35	Si	-1.539449	-4.088562	4.507120	-1.528071	-4.197988	4.632725	-1.521397	-4.169485	4.597461
36	Si	-1.689776	-4.101236	-2.355637	-1.669932	-4.146433	-2.380328	-1.668403	-4.123192	-2.367296
37	Si	-1.520896	-1.863768	-5.794307	-1.527433	-1.913340	-5.950688	-1.519615	-1.897017	-5.907939
38	Si	-1.509589	-5.852577	-5.639816	-1.617594	-5.927811	-5.705052	-1.602236	-5.896877	-5.677607
39	Si	-1.514300	-7.837013	-2.210114	-1.615786	-7.917594	-2.241969	-1.601228	-7.877867	-2.231134
40	Si	0.794723	5.814575	1.108018	0.838125	5.979126	1.135955	0.832402	5.937174	1.129850
41	Si	0.797098	-2.093473	7.803480	0.731985	-2.142139	7.973003	0.735210	-2.129571	7.926313
42	Si	0.788626	-3.862781	4.468726	0.838940	-3.973752	4.610755	0.832407	-3.947398	4.577267
43	Si	0.649966	3.972092	-2.297766	0.703242	4.101508	-2.381887	0.693157	4.068401	-2.361944
44	Si	0.815031	5.694181	-5.734150	0.731405	5.805884	-5.870579	0.735812	5.773552	-5.834413
45	Si	0.806802	1.917906	-5.583781	0.839206	1.975982	-5.755246	0.833925	1.962406	-5.715149
46	Si	0.797114	2.126541	7.794497	0.732014	2.182593	7.962348	0.735217	2.167123	7.916211
47	Si	0.806770	-1.941592	-5.575580	0.839181	-2.005319	-5.745443	0.833914	-1.989509	-5.705850
48	Si	0.630269	0.009714	4.580883	0.702709	0.012177	4.740458	0.691656	0.011189	4.701986
49	Si	0.788669	3.881718	4.452243	0.838947	3.997314	4.590908	0.832419	3.969113	4.558595
50	Si	0.794716	-5.809821	1.132698	0.838200	-5.973282	1.165925	0.832422	-5.931758	1.157903
51	Si	0.649904	-3.981816	-2.280864	0.703211	-4.113668	-2.361424	0.693136	-4.079581	-2.342709
52	Si	0.815015	-5.718415	-5.710010	0.731392	-5.835703	-5.841659	0.735805	-5.801161	-5.807121
53	Si	0.809978	7.820058	-2.090735	0.733472	7.977042	-2.131406	0.737026	7.930474	-2.118888
54	Si	0.809987	-7.828815	-2.057603	0.733564	-7.987820	-2.091267	0.737053	-7.940435	-2.081373
55	Si	1.662362	3.981818	2.281056	1.680070	4.113666	2.361563	1.672768	4.079588	2.342832
56	Si	1.517616	5.809839	-1.132588	1.545123	5.973255	-1.165847	1.533520	5.931749	-1.157845
57	Si	1.497199	5.718354	5.710370	1.651874	5.835676	5.841880	1.630085	5.801143	5.807330
58	Si	1.502277	7.828721	2.057959	1.649718	7.987770	2.091461	1.628852	7.940387	2.081556
59	Si	1.505101	1.941582	5.575773	1.543887	2.005319	5.745598	1.531794	1.989522	5.705982
60	Si	1.505079	-1.917908	5.583986	1.543863	-1.976000	5.755392	1.531784	-1.962409	5.715269
61	Si	1.497180	-5.694139	5.734501	1.651863	-5.805875	5.870794	1.630078	-5.773525	5.834609
62	Si	1.523535	3.862693	-4.468561	1.544291	3.973684	-4.610643	1.533450	3.947349	-4.577176
63	Si	1.681574	-0.009730	-4.580693	1.680355	-0.012184	-4.740306	1.674046	-0.011182	-4.701858
64	Si	1.514798	2.093494	-7.803252	1.651079	2.142117	-7.972847	1.630498	2.129571	-7.926183
65	Si	1.514773	-2.126562	-7.794288	1.651050	-2.182596	-7.962183	1.630488	-2.167119	-7.916069
66	Si	1.517607	-5.814578	-1.107908	1.545195	-5.979137	-1.135879	1.533538	-5.937177	-1.129790
67	Si	1.523491	-3.881630	-4.452088	1.544280	-3.997266	-4.590789	1.533436	-3.969054	-4.558491
68	Si	1.502292	-7.819951	2.091082	1.649815	-7.977030	2.131602	1.628882	-7.930439	2.119073
69	Si	1.662299	-3.972081	2.297970	1.680042	-4.101538	2.382018	1.672750	-4.068414	2.362053
70	Si	3.826614	-7.827768	2.242954	3.999206	-7.906136	2.281489	3.967188	-7.867296	2.268142
71	Si	4.002039	4.101320	2.355640	4.053209	4.146469	2.380360	4.034304	4.123227	2.367331
72	Si	3.845957	5.961171	-1.303307	3.911729	6.105043	-1.347243	3.887040	6.060616	-1.338652
73	Si	3.851628	4.088534	-4.507370	3.911316	4.197941	-4.632886	3.887267	4.169456	-4.597615
74	Si	3.821774	5.852754	5.639445	4.000836	5.927914	5.704849	3.968104	5.896981	5.677419
75	Si	4.021406	-0.010072	-4.724476	4.053218	-0.012179	-4.777496	4.035336	-0.011277	-4.751622
76	Si	3.839049	1.966250	-7.885356	4.000059	1.976593	-7.984522	3.968538	1.968733	-7.944560
77	Si	3.839028	-1.999663	-7.876903	4.000025	-2.017054	-7.974605	3.968529	-2.006341	-7.935187
78	Si	3.826607	7.837289	2.209695	3.999097	7.917742	2.241721	3.967159	7.878008	2.230905
79	Si	4.001982	-4.091168	2.373030	4.053199	-4.134267	2.400820	4.034290	-4.111915	2.386721

80	Si	3.845952	-5.966682	-1.277998	3.911822	-6.111865	-1.316719	3.887061	-6.066905	-1.310013
81	Si	3.832784	1.863681	5.794126	3.910505	1.913290	5.950599	3.885326	1.896981	5.907852
82	Si	3.851588	-4.107626	-4.489908	3.911312	-4.221687	-4.612013	3.887256	-4.191255	-4.577899
83	Si	3.832755	-1.839099	5.802047	3.910446	-1.882997	5.960097	3.885312	-1.868937	5.916744
84	Si	3.821762	-5.828756	5.664205	4.000831	-5.898765	5.734373	3.968099	-5.869964	5.705193
85	H	-5.136513	8.997931	-0.688991	-5.214011	9.140787	-0.643347	-5.181232	9.080635	-0.644843
86	H	-5.210546	7.317537	-4.245000	-5.245240	7.421088	-4.306906	-5.217553	7.382074	-4.283345
87	H	-5.145150	3.930282	8.097278	-5.214729	4.053462	8.215091	-5.182532	4.019527	8.165046
88	H	-5.124086	5.055762	-7.446642	-5.212286	5.088341	-7.619416	-5.179202	5.062146	-7.565052
89	H	-5.225831	0.018004	8.459719	-5.241652	0.021761	8.580383	-5.216129	0.020214	8.533854
90	H	-5.124134	-5.087263	-7.425043	-5.212344	-5.126857	-7.594083	-5.179205	-5.097924	-7.541101
91	H	-5.145217	-3.895943	8.113954	-5.214681	-4.011772	8.235293	-5.182519	-3.980804	8.183955
92	H	-5.210623	-7.335494	-4.213904	-5.245166	-7.443044	-4.269592	-5.217554	-7.402342	-4.248396
93	H	-5.136507	-9.000823	-0.650735	-5.213939	-9.143902	-0.597264	-5.181217	-9.083595	-0.601853
94	H	-1.812432	5.087305	7.424594	-1.937312	5.126944	7.593764	-1.918404	5.097971	7.540819
95	H	-1.725551	7.335583	4.213618	-1.904267	7.443156	4.269362	-1.879853	7.402413	4.248196
96	H	-1.799503	9.000768	0.650083	-1.935423	9.143910	0.596826	-1.916121	9.083571	0.601460
97	H	-1.791326	3.895841	-8.114526	-1.934933	4.011748	-8.235652	-1.915054	3.980755	-8.184286
98	H	-1.812476	-5.055818	7.446180	-1.937370	-5.088351	7.619087	-1.918406	-5.062181	7.564751
99	H	-1.725623	-7.317601	4.244715	-1.904187	-7.421140	4.306682	-1.879851	-7.382142	4.283142
100	H	-1.799491	-8.997868	0.688322	-1.935349	-9.140746	0.642908	-1.916103	-9.080622	0.644447
101	H	-1.791397	-3.930163	-8.097860	-1.934891	-4.053358	-8.215441	-1.915047	-4.019461	-8.165364
102	H	-1.710940	-0.018010	-8.459890	-1.908098	-0.021727	-8.580477	-1.881567	-0.020215	-8.533941
103	H	-2.028936	2.152705	9.292798	-2.140117	2.138412	9.384688	-2.120696	2.131153	9.334766
104	H	-2.015851	9.123455	-2.833981	-2.136984	9.185961	-2.887353	-2.117647	9.139605	-2.865654
105	H	-2.239969	2.885788	-3.085927	-2.183691	2.897640	-3.072276	-2.184211	2.889120	-3.057155
106	H	-2.249819	4.081670	-0.976646	-2.184727	4.100568	-0.994551	-2.183829	4.085613	-0.992373
107	H	-2.011128	6.977479	-6.506249	-2.139813	7.058140	-6.546706	-2.119450	7.018659	-6.514929
108	H	-2.200212	4.693099	0.820345	-2.112764	4.809731	0.845818	-2.108968	4.773526	0.854994
109	H	-2.187428	1.590081	-4.472234	-2.110562	1.644771	-4.595745	-2.106207	1.621554	-4.567715
110	H	-2.202455	3.077158	3.609910	-2.111343	3.158590	3.723947	-2.108466	3.146581	3.689236
111	H	-2.028946	-2.113235	9.301917	-2.140134	-2.090958	9.395182	-2.120700	-2.086930	9.344704
112	H	-2.265619	1.220884	4.025761	-2.183729	1.210796	4.040650	-2.184767	1.202831	4.027023
113	H	-2.265669	-1.203736	4.030808	-2.183496	-1.190479	4.047104	-2.184687	-1.183810	4.032782
114	H	-2.200201	-4.689512	0.840289	-2.112680	-4.805381	0.869680	-2.108936	-4.769422	0.877477
115	H	-2.202497	-3.061736	3.623052	-2.111252	-3.139417	3.739316	-2.108477	-3.129021	3.703967
116	H	-2.249911	-4.085905	-0.959350	-2.184969	-4.105297	-0.974341	-2.183904	-4.090246	-0.973128
117	H	-2.240021	-2.898962	-3.073694	-2.183471	-2.913469	-3.058558	-2.184187	-2.903676	-3.043645
118	H	-2.187405	-1.609010	-4.465348	-2.110494	-1.668225	-4.587398	-2.106188	-1.643187	-4.559987
119	H	-2.011140	-7.004998	-6.476677	-2.139909	-7.091371	-6.511290	-2.119478	-7.049467	-6.481711
120	H	-2.015821	-9.135486	-2.795169	-2.136845	-9.200692	-2.841035	-2.117602	-9.153159	-2.822361
121	H	1.229863	-3.437606	8.330942	1.109019	-3.483485	8.537764	1.114350	-3.462411	8.481302
122	H	1.471592	-1.035686	8.638337	1.382999	-1.101018	8.838297	1.383991	-1.093209	8.780188
123	H	1.072040	2.719811	-1.564490	1.158336	2.856961	-1.660520	1.141374	2.832369	-1.645194
124	H	1.490805	6.945400	-5.235588	1.381368	7.076823	-5.403215	1.383950	7.032271	-5.366011
125	H	1.247479	5.477990	-7.161837	1.109494	5.621982	-7.314011	1.115519	5.585027	-7.265653
126	H	1.471606	1.072308	8.633839	1.383006	1.145921	8.832987	1.383999	1.134837	8.775009
127	H	1.229833	3.472895	8.316297	1.108960	3.526794	8.520360	1.114321	3.502584	8.464886

128	H	1.050405	0.006622	3.129161	1.158688	0.008652	3.302203	1.140656	0.007833	3.273424
129	H	1.071946	-2.726420	-1.552921	1.158287	-2.865399	-1.646512	1.141343	-2.840142	-1.631864
130	H	1.247389	-5.508111	-7.138600	1.109362	-5.658763	-7.285989	1.115484	-5.619328	-7.239233
131	H	1.490852	-6.967548	-5.206331	1.381424	-7.104385	-5.368261	1.383961	-7.057677	-5.332858
132	H	1.242945	8.947678	-1.188996	1.109544	9.137699	-1.252880	1.115301	9.078145	-1.242515
133	H	1.485071	8.014965	-3.423720	1.386572	8.204304	-3.464980	1.387430	8.150665	-3.442775
134	H	1.485012	-8.029238	-3.389809	1.386679	-8.221796	-3.423673	1.387440	-8.166849	-3.404219
135	H	1.243082	-8.952635	-1.151191	1.109655	-9.144022	-1.206886	1.115365	-9.083954	-1.199605
136	H	1.240279	2.726390	1.553197	1.224969	2.865378	1.646704	1.224539	2.840127	1.632039
137	H	1.065584	5.507472	7.139107	1.274317	5.658413	7.286283	1.250802	5.618992	7.239509
138	H	0.820829	6.967500	5.207455	1.001562	7.104374	5.368914	0.981663	7.057679	5.333491
139	H	0.827926	8.028416	3.390620	0.996951	8.221351	3.424108	0.978796	8.166409	3.404635
140	H	1.068384	8.952790	1.152253	1.273212	9.144114	1.207449	1.250142	9.084052	1.200154
141	H	0.820894	-6.945366	5.236666	1.001627	-7.076830	5.403856	0.981677	-7.032262	5.366623
142	H	1.065465	-5.477403	7.162330	1.274182	-5.621657	7.314294	1.250762	-5.584687	7.265913
143	H	1.261525	-0.006639	-3.128942	1.224438	-0.008656	-3.302028	1.225098	-0.007822	-3.273279
144	H	1.082069	3.437700	-8.330569	1.274041	3.483494	-8.537540	1.251362	3.462444	-8.481099
145	H	0.840163	1.035813	-8.638131	0.999991	1.101035	-8.838134	0.981645	1.093254	-8.780058
146	H	0.840149	-1.072423	-8.633645	0.999976	-1.145976	-8.832822	0.981631	-1.134884	-8.774871
147	H	1.082081	-3.472981	-8.315953	1.274112	-3.526831	-8.520116	1.251392	-3.502616	-8.464668
148	H	1.068543	-8.947814	1.190033	1.273333	-9.137830	1.253444	1.250212	-9.078255	1.243067
149	H	0.827858	-8.014144	3.424512	0.997060	-8.203899	3.465415	0.978808	-8.150238	3.443191
150	H	1.240181	-2.719771	1.564775	1.224923	-2.856977	1.660695	1.224510	-2.832367	1.645346
151	H	4.328166	-9.123685	2.833626	4.520315	-9.186123	2.887137	4.483590	-9.139739	2.865455
152	H	4.552414	2.899270	3.073979	4.566822	2.913643	3.058789	4.550148	2.903845	3.043880
153	H	4.562078	4.085674	0.959317	4.568191	4.105121	0.974360	4.549763	4.090071	0.973152
154	H	4.512577	4.689590	-0.840346	4.496043	4.805402	-0.869718	4.474912	4.769452	-0.877516
155	H	4.514913	3.061745	-3.623436	4.494638	3.139370	-3.739566	4.474477	3.128997	-3.704202
156	H	4.323486	7.004948	6.476526	4.523242	7.091340	6.511225	4.485435	7.049450	6.481644
157	H	4.577519	1.203628	-4.030594	4.566560	1.190459	-4.046982	4.550396	1.183777	-4.032663
158	H	4.577413	-1.220967	-4.025623	4.566789	-1.210796	-4.040542	4.550452	-1.202846	-4.026939
159	H	4.340659	2.112914	-9.301995	4.523083	2.090746	-9.395239	4.486305	2.086745	-9.344761
160	H	4.340652	-2.152389	-9.292897	4.523063	-2.138220	-9.384734	4.486297	-2.130972	-9.334814
161	H	4.328128	9.135732	2.794812	4.520167	9.200823	2.840815	4.483538	9.153288	2.822155
162	H	4.562001	-4.081376	0.976648	4.567954	-4.100436	0.994555	4.549692	-4.085447	0.992380
163	H	4.552336	-2.886079	3.086274	4.567043	-2.897847	3.072488	4.550170	-2.889295	3.057371
164	H	4.512586	-4.693172	-0.820397	4.496118	-4.809777	-0.845849	4.474937	-4.773564	-0.855018
165	H	4.498976	1.608671	4.465063	4.493369	1.668017	4.587255	4.471719	1.643009	4.559851
166	H	4.514857	-3.077115	-3.610301	4.494723	-3.158572	-3.724178	4.474465	-3.146557	-3.689445
167	H	4.498996	-1.589744	4.471935	4.493438	-1.644569	4.595598	4.471741	-1.621352	4.567570
168	H	4.323480	-6.977433	6.506103	4.523149	-7.058117	6.546647	4.485406	-7.018628	6.514860
169	Tv	9.248491	0.000000	0.000000	9.532750	-0.000039	0.000003	9.463342	0.000000	0.000000

	Atomic Type	SiNW [111] - LDA			SiNW [111] - GGA			SiNW [111] - HSE		
		x	y	z	x	y	z	x	y	z
1	Si	-4.252718	7.657348	0.000000	-4.312405	7.743616	0.000000	-4.289326	7.705237	0.000000
2	Si	-4.237990	5.729389	-3.322575	-4.297663	5.790785	-3.359800	-4.274784	5.763596	-3.342713
3	Si	-4.251342	3.853450	6.618545	-4.310869	3.899568	6.691533	-4.288079	3.878074	6.659358

4	Si	-4.253880	3.803818	-6.647348	-4.313697	3.843890	-6.723812	-4.290390	3.826991	-6.688986
5	Si	-4.279473	5.771706	3.318072	-4.344534	5.836627	3.353877	-4.320355	5.805511	3.337195
6	Si	-4.256391	3.833138	-0.006250	-4.323338	3.882640	-0.007706	-4.299014	3.861971	-0.007089
7	Si	-4.256816	1.909685	-3.324709	-4.323924	1.934069	-3.367703	-4.299484	1.924340	-3.349265
8	Si	-4.256950	1.923719	3.316502	-4.322735	1.948821	3.359015	-4.298530	1.937825	3.341334
9	Si	-4.235649	0.012501	6.624281	-4.295496	0.014088	6.696252	-4.272990	0.012903	6.663924
10	Si	-4.281855	-0.012585	-6.658635	-4.346854	-0.014174	-6.732963	-4.322285	-0.012975	-6.697503
11	Si	-4.257927	-0.000008	-0.000153	-4.323333	-0.000002	-0.000124	-4.299145	-0.000001	-0.000103
12	Si	-4.255919	-1.911177	3.323677	-4.322709	-1.934661	3.367135	-4.298508	-1.924865	3.348770
13	Si	-4.256786	-1.922252	-3.317523	-4.323898	-1.948237	-3.359582	-4.299463	-1.937307	-3.341828
14	Si	-4.256323	-3.833129	0.008119	-4.323284	-3.882639	0.008542	-4.298970	-3.861970	0.007791
15	Si	-4.237890	-5.741888	-3.301091	-4.297581	-5.804871	-3.335559	-4.274713	-5.776496	-3.320504
16	Si	-4.253814	-3.828908	-6.633063	-4.313639	-3.872164	-6.707689	-4.290338	-3.852876	-6.674216
17	Si	-4.251275	-3.828432	6.632902	-4.310814	-3.871368	6.707773	-4.288029	-3.852252	6.674232
18	Si	-4.279367	-5.759114	3.339639	-4.344451	-5.822454	3.378246	-4.320284	-5.792539	3.359516
19	Si	-4.252575	-7.657264	0.028662	-4.312301	-7.743537	0.032379	-4.289242	-7.705171	0.029664
20	Si	-1.912314	1.922240	3.317303	-1.942477	1.948233	3.359422	-1.931693	1.937304	3.341683
21	Si	-1.915283	3.828908	6.632781	-1.952735	3.872160	6.707475	-1.940816	3.852874	6.674022
22	Si	-1.887259	0.012575	6.658458	-1.919535	0.014176	6.732830	-1.908888	0.012978	6.697373
23	Si	-1.889723	5.759037	-3.339974	-1.921916	5.822402	-3.378468	-1.910859	5.792496	-3.359720
24	Si	-1.931212	5.741895	3.300793	-1.968793	5.804869	3.335344	-1.956437	5.776493	3.320313
25	Si	-1.912285	-1.909688	3.324474	-1.942451	-1.934061	3.367542	-1.931671	-1.924335	3.349120
26	Si	-1.912769	3.833117	-0.008378	-1.943087	3.882628	-0.008717	-1.932178	3.861963	-0.007948
27	Si	-1.917802	3.828371	-6.633297	-1.955548	3.871341	-6.708049	-1.943116	3.852225	-6.674477
28	Si	-1.916563	7.657232	-0.029051	-1.954102	7.743506	-0.032642	-1.941928	7.705145	-0.029902
29	Si	-1.931110	-5.729385	3.322257	-1.968711	-5.790778	3.359585	-1.956366	-5.763590	3.342523
30	Si	-1.912703	-3.833116	0.005993	-1.943033	-3.882626	0.007530	-1.932133	-3.861961	0.006931
31	Si	-1.913162	-1.923705	-3.316758	-1.943647	-1.948809	-3.359200	-1.932631	-1.937814	-3.341497
32	Si	-1.889623	-5.771611	-3.318386	-1.921833	-5.836572	-3.354101	-1.910788	-5.805466	-3.337401
33	Si	-1.911175	-0.000003	-0.000102	-1.943044	0.000003	-0.000050	-1.932010	0.000003	-0.000053
34	Si	-1.913191	1.911148	-3.323947	-1.943673	1.934652	-3.367319	-1.932652	1.924857	-3.348933
35	Si	-1.915215	-3.803825	6.647040	-1.952678	-3.843883	6.723596	-1.940765	-3.826985	6.688793
36	Si	-1.917740	-3.853400	-6.618917	-1.955492	-3.899539	-6.691809	-1.943067	-3.878044	-6.659604
37	Si	-1.916423	-7.657281	-0.000391	-1.953998	-7.743580	-0.000264	-1.941846	-7.705208	-0.000238
38	Si	-1.933451	-0.012513	-6.624586	-1.970882	-0.014087	-6.696474	-1.958171	-0.012901	-6.664122
39	Si	-1.102282	1.936180	7.741264	-1.130865	1.961586	7.829077	-1.124885	1.950183	7.790172
40	Si	-1.103271	7.662180	-2.222497	-1.132180	7.749932	-2.248267	-1.125992	7.711590	-2.235941
41	Si	-1.144131	1.909393	-5.537861	-1.156437	1.931337	-5.608417	-1.149918	1.921833	-5.578484
42	Si	-1.132045	1.919165	1.103621	-1.149893	1.943837	1.117229	-1.143491	1.933351	1.111570
43	Si	-1.142442	3.840126	4.422945	-1.154427	3.890480	4.477323	-1.148285	3.869444	4.454059
44	Si	-1.143052	5.753480	1.092759	-1.155121	5.826297	1.106400	-1.148831	5.795438	1.101869
45	Si	-1.102247	-1.906949	7.748450	-1.130835	-1.928618	7.837209	-1.124858	-1.919994	7.797617
46	Si	-1.136333	3.835984	-2.224896	-1.149373	3.880239	-2.251582	-1.143028	3.859949	-2.238864
47	Si	-1.104887	5.734122	-5.547166	-1.134020	5.797475	-5.613216	-1.127490	5.769763	-5.583872
48	Si	-1.132637	-0.004198	-2.214129	-1.150573	-0.004726	-2.242250	-1.144031	-0.004324	-2.230297
49	Si	-1.135015	0.008370	4.435194	-1.148064	0.009445	4.487058	-1.141987	0.008645	4.463000
50	Si	-1.136278	-3.844384	-2.210499	-1.149329	-3.889699	-2.235331	-1.142991	-3.868605	-2.223981
51	Si	-1.144104	-1.930319	-5.530668	-1.156412	-1.954937	-5.600298	-1.149896	-1.943433	-5.571049

52	Si	-1.132013	-1.914996	1.110804	-1.149869	-1.939120	1.125352	-1.143470	-1.929032	1.119009
53	Si	-1.104801	-5.755042	-5.525654	-1.133940	-5.821059	-5.588932	-1.127423	-5.791354	-5.561623
54	Si	-1.142940	-5.749330	1.114289	-1.155033	-5.821608	1.130748	-1.148758	-5.791143	1.124167
55	Si	-1.142372	-3.823405	4.437264	-1.154373	-3.871607	4.493539	-1.148236	-3.852169	4.468909
56	Si	-1.103104	-7.670519	-2.193784	-1.132059	-7.759332	-2.215834	-1.125893	-7.720197	-2.206228
57	Si	1.200344	5.749702	1.092448	1.222229	5.831273	1.106670	1.215397	5.799463	1.101827
58	Si	1.230686	2.088741	7.729250	1.225279	2.123418	7.828335	1.220644	2.110433	7.788394
59	Si	1.212812	1.925000	1.106853	1.229470	1.951088	1.121266	1.222603	1.940137	1.115342
60	Si	1.201039	3.837220	4.420097	1.223011	3.892719	4.481487	1.216019	3.871009	4.457539
61	Si	1.212838	-1.920799	1.114052	1.229491	-1.946334	1.129417	1.222621	-1.935789	1.122806
62	Si	1.199417	-1.928980	-5.527446	1.221054	-1.957510	-5.604797	1.214431	-1.945711	-5.574588
63	Si	1.209928	0.008389	4.441415	1.229802	0.009479	4.501225	1.222654	0.008674	4.476228
64	Si	1.230728	-2.059502	7.737034	1.225315	-2.090406	7.837162	1.220675	-2.080182	7.796475
65	Si	1.201100	-3.820489	4.434432	1.223061	-3.873813	4.497732	1.216061	-3.853711	4.472414
66	Si	1.208650	3.840996	-2.228011	1.228481	3.892334	-2.258727	1.221605	3.871300	-2.245583
67	Si	1.228309	5.647992	-5.672016	1.222272	5.717317	-5.751224	1.218150	5.689262	-5.720313
68	Si	1.199390	1.908077	-5.534635	1.221028	1.933903	-5.612929	1.214408	1.924108	-5.582029
69	Si	1.212141	-0.004206	-2.221124	1.228778	-0.004741	-2.250917	1.222053	-0.004338	-2.238380
70	Si	1.208702	-3.849397	-2.213601	1.228523	-3.901817	-2.242428	1.221640	-3.879976	-2.230661
71	Si	1.228390	-5.669398	-5.650783	1.222353	-5.741505	-5.727223	1.218219	-5.711414	-5.698306
72	Si	1.200457	-5.745536	1.113990	1.222322	-5.826568	1.131057	1.215474	-5.795154	1.124152
73	Si	1.229844	7.728721	-2.083801	1.224165	7.831073	-2.107917	1.219682	7.791030	-2.096362
74	Si	1.230003	-7.736535	-2.054755	1.224282	-7.839899	-2.075039	1.219775	-7.799121	-2.066236
75	Si	1.999346	1.928981	5.527556	2.028158	1.957515	5.604876	2.016517	1.945715	5.574634
76	Si	1.999374	-1.908104	5.534734	2.028184	-1.933909	5.613007	2.016539	-1.924114	5.582077
77	Si	1.970462	5.669151	5.651352	2.026933	5.741341	5.727599	2.012793	5.711257	5.698643
78	Si	1.968760	7.736286	2.055392	2.024936	7.839717	2.075485	2.011185	7.798934	2.066654
79	Si	1.990091	3.849404	2.213675	2.020710	3.901818	2.242487	2.009331	3.879976	2.230695
80	Si	1.998354	5.745540	-1.113952	2.026924	5.826571	-1.131015	2.015510	5.795160	-1.124138
81	Si	1.985954	1.920787	-1.113990	2.019741	1.946336	-1.129360	2.008349	1.935791	-1.122773
82	Si	1.988860	-0.008404	-4.441338	2.019427	-0.009480	-4.501167	2.008311	-0.008675	-4.476197
83	Si	1.968067	-2.088833	-7.729094	2.023916	-2.123494	-7.828224	2.010292	-2.110524	-7.788317
84	Si	1.985983	-1.925014	-1.106785	2.019763	-1.951091	-1.121208	2.008367	-1.940141	-1.115308
85	Si	1.998466	-5.749696	-1.092404	2.027016	-5.831278	-1.106628	2.015588	-5.799470	-1.101811
86	Si	1.997767	-3.837177	-4.419994	2.026232	-3.892690	-4.481413	2.014957	-3.870982	-4.457495
87	Si	1.970558	-5.647748	5.672552	2.027013	-5.717158	5.751595	2.012864	-5.689108	5.720645
88	Si	1.968023	2.059561	-7.736893	2.023880	2.090473	-7.837053	2.010259	2.080265	-7.796398
89	Si	1.986656	0.004188	2.221185	2.020457	0.004740	2.250969	2.008918	0.004337	2.238408
90	Si	1.997709	3.820433	-4.434351	2.026183	3.873782	-4.497659	2.014915	3.853682	-4.472370
91	Si	1.990145	-3.841007	2.228073	2.020752	-3.892336	2.258786	2.009367	-3.871301	2.245616
92	Si	1.968937	-7.728449	2.084425	2.025053	-7.830893	2.108361	2.011278	-7.790844	2.096779
93	Si	4.342874	1.930327	5.530425	4.405626	1.954944	5.600118	4.380847	1.943440	5.570885
94	Si	4.342902	-1.909415	5.537601	4.405651	-1.931342	5.608237	4.380868	-1.921838	5.578322
95	Si	4.331436	0.004187	2.213895	4.399808	0.004727	2.242090	4.375004	0.004325	2.230152
96	Si	4.333805	-0.008384	-4.435360	4.397296	-0.009444	-4.487177	4.372954	-0.008644	-4.463114
97	Si	4.300975	1.906905	-7.748591	4.380013	1.928603	-7.837307	4.355778	1.919987	-7.797718
98	Si	4.301009	-1.936160	-7.741393	4.380044	-1.961568	-7.829176	4.355803	-1.950173	-7.790273
99	Si	4.335127	-3.836023	2.224652	4.398605	-3.880263	2.251424	4.373998	-3.859968	2.238720

100	Si	4.303617	5.755159	5.525380	4.383195	5.821135	5.588730	4.358409	5.791422	5.561431
101	Si	4.330835	-1.919184	-1.103833	4.399126	-1.943845	-1.117374	4.374459	-1.933357	-1.111702
102	Si	4.341848	-5.753464	-1.093036	4.404357	-5.826295	-1.106589	4.379807	-5.795435	-1.102039
103	Si	4.341252	-3.840114	-4.423188	4.403676	-3.890474	-4.477501	4.379266	-3.869441	-4.454222
104	Si	4.301936	7.670626	2.193454	4.381321	7.759393	2.215609	4.356894	7.720245	2.206020
105	Si	4.303710	-5.734235	5.546862	4.383275	-5.797550	5.613016	4.358478	-5.769830	5.583682
106	Si	4.302108	-7.662262	2.222153	4.381443	-7.749993	2.248044	4.356993	-7.711637	2.235734
107	Si	4.335073	3.844428	2.210274	4.398562	3.889724	2.235172	4.373962	3.868625	2.223835
108	Si	4.341739	5.749336	-1.114571	4.404269	5.821608	-1.130938	4.379733	5.791142	-1.124337
109	Si	4.330806	1.915001	-1.111020	4.399101	1.939130	-1.125496	4.374439	1.929040	-1.119142
110	Si	4.341186	3.823388	-4.437528	4.403620	3.871603	-4.493717	4.379218	3.852168	-4.469071
111	H	-4.778011	8.868702	-0.736461	-4.818517	8.966472	-0.725951	-4.792801	8.918309	-0.720951
112	H	-4.768063	6.956033	-4.032754	-4.800897	7.022615	-4.073252	-4.775370	6.985923	-4.050643
113	H	-4.777287	3.827365	8.035718	-4.817238	3.888554	8.113501	-4.791985	3.865982	8.070286
114	H	-4.778842	5.044565	-7.333367	-4.819679	5.081067	-7.425185	-4.793710	5.055251	-7.383876
115	H	-4.766377	0.015153	8.041395	-4.799866	0.017055	8.119453	-4.774713	0.015612	8.076117
116	H	-4.768002	-6.971182	-4.006602	-4.800838	-7.039687	-4.043814	-4.775315	-7.001558	-4.023681
117	H	-4.778810	-5.072231	-7.314356	-4.819647	-5.112279	-7.403835	-4.793677	-5.083822	-7.364322
118	H	-4.777212	-3.797044	8.049963	-4.817187	-3.854403	8.129683	-4.791935	-3.834727	8.085104
119	H	-4.777906	-8.871370	-0.703186	-4.818439	-8.969429	-0.688414	-4.792740	-8.921024	-0.686570
120	H	-1.390270	5.072331	7.313921	-1.446720	5.112337	7.403509	-1.437464	5.083870	7.364046
121	H	-1.401030	6.971270	4.006163	-1.465493	7.039731	4.043487	-1.455800	7.001593	4.023406
122	H	-1.391961	3.796933	-8.050397	-1.449233	3.854345	-8.129979	-1.439265	3.834665	-8.085363
123	H	-1.391143	8.871444	0.702590	-1.447918	8.969461	0.688003	-1.438393	8.921053	0.686209
124	H	-1.400981	-6.956076	4.032280	-1.465433	-7.022656	4.072925	-1.455743	-6.985954	4.050369
125	H	-1.390245	-5.044653	7.332896	-1.446688	-5.081119	7.424861	-1.437431	-5.055292	7.383601
126	H	-1.391900	-3.827261	-8.036115	-1.449183	-3.888489	-8.113798	-1.439215	-3.865914	-8.070547
127	H	-1.391058	-8.868711	0.735848	-1.447838	-8.966499	0.725542	-1.438332	-8.918333	0.720592
128	H	-1.402844	-0.015162	-8.041735	-1.466588	-0.017051	-8.119700	-1.456509	-0.015610	-8.076330
129	H	-1.626872	1.929597	9.157926	-1.649130	1.957468	9.246750	-1.639929	1.945158	9.196917
130	H	-1.627473	8.883387	-2.940913	-1.650613	8.972755	-2.965483	-1.641009	8.924755	-2.948161
131	H	-1.626851	-1.895087	9.165071	-1.649110	-1.918586	9.254850	-1.639910	-1.909573	9.204331
132	H	-1.628546	6.965022	-6.249236	-1.651874	7.027906	-6.317706	-1.642005	6.991136	-6.282286
133	H	-1.628468	-6.988586	-6.223034	-1.651807	-7.054449	-6.288218	-1.641946	-7.015433	-6.255278
134	H	-1.627303	-8.894435	-2.907541	-1.650486	-8.985175	-2.927877	-1.640906	-8.936126	-2.913721
135	H	1.879069	1.048915	8.604242	1.862523	1.099817	8.721796	1.854405	1.093038	8.673141
136	H	1.622184	3.443969	8.261697	1.599502	3.472817	8.375549	1.591993	3.452128	8.327290
137	H	1.622244	-3.412684	8.274620	1.599550	-3.437477	8.390075	1.592066	-3.419736	8.340638
138	H	1.879096	-1.016348	8.608077	1.862553	-1.063027	8.726292	1.854404	-1.059294	8.677215
139	H	1.875314	6.925479	-5.206603	1.856206	7.003171	-5.307750	1.849304	6.964261	-5.278273
140	H	1.621569	5.433839	-7.111727	1.599140	5.520195	-7.193229	1.591687	5.488358	-7.151558
141	H	1.621689	-5.460676	-7.091268	1.599272	-5.550468	-7.170032	1.591829	-5.516118	-7.130308
142	H	1.875348	-6.945148	-5.180603	1.856248	-7.025504	-5.278341	1.849314	-6.984708	-5.251279
143	H	1.620392	8.870334	-1.179605	1.597589	8.983348	-1.217348	1.590211	8.931938	-1.207863
144	H	1.878915	7.962727	-3.422153	1.861961	8.088093	-3.441881	1.853916	8.044047	-3.420513
145	H	1.879158	-7.975603	-3.392154	1.862172	-8.102632	-3.407846	1.854098	-8.057394	-3.389329
146	H	1.620495	-8.874675	-1.146200	1.597806	-8.988364	-1.179519	1.590204	-8.936511	-1.173194
147	H	1.578053	5.459434	7.091967	1.650611	5.549648	7.170486	1.639751	5.515320	7.130715

148	H	1.322871	6.945039	5.182366	1.392620	7.025422	5.279531	1.381294	6.984632	5.252402
149	H	1.320379	7.974174	3.393414	1.387573	8.101642	3.408709	1.377369	8.056398	3.390158
150	H	1.577372	8.875005	1.147936	1.651011	8.988570	1.180724	1.640170	8.936714	1.174363
151	H	1.319504	-1.049158	-8.604109	1.386542	-1.100005	-8.721709	1.376410	-1.093260	-8.673104
152	H	1.576595	-3.444153	-8.261285	1.649715	-3.472974	-8.375248	1.638976	-3.452303	-8.327014
153	H	1.322947	-6.925340	5.208334	1.392667	-7.003090	5.308931	1.381311	-6.964185	5.279384
154	H	1.578185	-5.432630	7.112369	1.650740	-5.519386	7.193676	1.639888	-5.487572	7.151959
155	H	1.576513	3.412838	-8.274246	1.649653	3.437617	-8.389787	1.638891	3.419897	-8.340374
156	H	1.319485	1.016532	-8.607940	1.386521	1.063193	-8.726196	1.376418	1.059494	-8.677171
157	H	1.577506	-8.870614	1.181361	1.651033	-8.983552	1.218548	1.640167	-8.932139	1.209031
158	H	1.320659	-7.961282	3.423360	1.387783	-8.087109	3.442737	1.377551	-8.043056	3.421335
159	H	4.825428	1.894992	-9.165250	4.898178	1.918535	-9.254975	4.870734	1.909539	-9.204453
160	H	4.825448	-1.929531	-9.158087	4.898199	-1.957417	-9.246876	4.870753	-1.945123	-9.197040
161	H	4.827381	6.988617	6.222893	4.901130	7.054454	6.288104	4.872995	7.015444	6.255159
162	H	4.826199	8.894490	2.907305	4.899789	8.985190	2.927710	4.871940	8.936137	2.913564
163	H	4.827458	-6.965028	6.249051	4.901199	-7.027909	6.317593	4.873057	-6.991146	6.282168
164	H	4.826368	-8.883388	2.940644	4.899919	-8.972769	2.965316	4.872045	-8.924765	2.948003
165	Tv	9.367895	0.000000	0.000000	9.515609	0.000000	0.000000	9.462124	0.000000	0.000000

	Atomic Type	SINT [112] - LDA			SINT [112] - GGA			SINT [112] - HSE		
		x	y	z	x	y	z	x	y	z
1	Si	-2.472513	7.979588	0.011983	-2.517712	8.081229	0.018889	-2.501540	8.037115	0.017840
2	Si	-2.448248	7.189243	-2.192182	-2.492788	7.306158	-2.219129	-2.478525	7.262927	-2.208609
3	Si	-2.422953	4.410114	1.247941	-2.468470	4.487624	1.273035	-2.452582	4.458725	1.263694
4	Si	-2.506427	0.900304	2.722388	-2.559415	0.918836	2.781488	-2.543905	0.912170	2.762380
5	Si	-2.380220	3.623066	-0.957394	-2.434166	3.736069	-0.982890	-2.418521	3.702928	-0.977376
6	Si	-2.425415	-2.801991	3.623200	-2.470869	-2.849796	3.689763	-2.454695	-2.832328	3.665690
7	Si	-2.475448	-6.405617	4.752922	-2.520703	-6.484382	4.818316	-2.504331	-6.449818	4.791774
8	Si	-2.384457	-3.483403	1.382699	-2.436939	-3.588390	1.429334	-2.421066	-3.558452	1.414612
9	Si	-2.478602	1.473737	-7.817314	-2.523668	1.486089	-7.924061	-2.508460	1.478277	-7.886957
10	Si	-2.452130	-7.083247	2.511609	-2.496275	-7.193258	2.558589	-2.481735	-7.152269	2.541782
11	Si	-2.477989	-5.841054	-5.408740	-2.523647	-5.910254	-5.488496	-2.508689	-5.881828	-5.462984
12	Si	-2.464265	-2.203361	-6.676363	-2.502581	-2.232685	-6.769884	-2.487609	-2.222571	-6.739420
13	Si	-1.264870	7.407301	3.575007	-1.278131	7.511330	3.641749	-1.271689	7.470286	3.622697
14	Si	-1.342568	6.475405	1.410223	-1.358376	6.575842	1.442500	-1.351194	6.536788	1.434374
15	Si	-1.625177	3.714633	5.027554	-1.652660	3.762159	5.103876	-1.645999	3.742915	5.076793
16	Si	-1.624553	0.003256	6.246118	-1.652229	0.010297	6.337702	-1.645687	0.009601	6.305082
17	Si	-1.398712	4.277212	-5.432375	-1.442877	4.330107	-5.511742	-1.431943	4.305771	-5.484292
18	Si	-1.406551	2.973795	2.795633	-1.433754	3.017769	2.836751	-1.425316	3.000593	2.821930
19	Si	-1.406773	-0.727120	4.010318	-1.434263	-0.738640	4.071735	-1.425831	-0.733790	4.050337
20	Si	-1.266647	-3.828198	7.277577	-1.280874	-3.872562	7.393458	-1.273817	-3.851345	7.354123
21	Si	-1.394959	0.602451	-4.286138	-1.420100	0.607330	-4.368491	-1.411814	0.603061	-4.345545
22	Si	-1.396372	-3.037177	-3.090511	-1.421724	-3.087944	-3.152506	-1.413150	-3.070767	-3.136691
23	Si	-1.344951	-4.365304	4.982701	-1.361085	-4.427971	5.068461	-1.353679	-4.401624	5.039204
24	Si	-1.399672	-6.672192	-1.822310	-1.444795	-6.760926	-1.856686	-1.433639	-6.724701	-1.848927
25	Si	-1.372175	-0.125573	-6.516307	-1.381669	-0.130906	-6.624907	-1.374813	-0.130536	-6.591109
26	Si	-1.632726	3.652520	-7.674166	-1.671290	3.690414	-7.781597	-1.660189	3.672420	-7.744194
27	Si	-1.371932	-3.781424	-5.315194	-1.381623	-3.837914	-5.405073	-1.374867	-3.818018	-5.377760



28	Si	-1.634566	-7.505717	-3.994713	-1.673970	-7.597170	-4.061397	-1.662611	-7.560317	-4.041816
29	Si	-0.522636	2.086729	6.330741	-0.518981	2.115818	6.419116	-0.521052	2.105796	6.388886
30	Si	-1.287864	6.009518	5.474998	-1.308802	6.089197	5.559829	-1.306239	6.057922	5.533886
31	Si	-0.248836	3.357008	-1.907639	-0.279551	3.453255	-1.944976	-0.273124	3.424851	-1.933126
32	Si	-0.251893	6.307923	-5.213966	-0.269368	6.377490	-5.276832	-0.266947	6.344599	-5.250775
33	Si	-0.251327	6.971653	-2.973660	-0.277464	7.073731	-3.017981	-0.272870	7.034420	-3.001922
34	Si	-1.289251	-1.574276	7.972186	-1.309643	-1.588513	8.088864	-1.307230	-1.579123	8.049863
35	Si	-0.252894	-3.833417	0.460430	-0.282086	-3.933123	0.487847	-0.275530	-3.902909	0.480713
36	Si	-0.290491	2.671584	-4.146724	-0.304682	2.711376	-4.204755	-0.302211	2.695040	-4.183590
37	Si	-0.252076	-0.995255	-3.011387	-0.261792	-1.018515	-3.085472	-0.259702	-1.012246	-3.066787
38	Si	-0.291523	-4.616894	-1.746741	-0.306221	-4.682691	-1.769821	-0.303611	-4.656574	-1.762240
39	Si	-0.252822	-8.174867	-0.438634	-0.271304	-8.267590	-0.450314	-0.268761	-8.225197	-0.448670
40	Si	-0.254578	-7.372812	1.755932	-0.280783	-7.481857	1.779087	-0.275916	-7.440386	1.768883
41	Si	0.836806	6.179575	0.570373	0.856968	6.274177	0.591997	0.851751	6.237521	0.587831
42	Si	0.871741	5.402631	-1.645727	0.881990	5.507447	-1.666893	0.877402	5.472288	-1.658096
43	Si	0.788867	-0.908162	3.177012	0.811865	-0.912027	3.261281	0.804941	-0.907419	3.237854
44	Si	0.787754	2.624716	2.015243	0.811776	2.676225	2.080396	0.804933	2.657577	2.064118
45	Si	0.834242	-4.625380	4.131342	0.854209	-4.689867	4.204897	0.849198	-4.663487	4.180268
46	Si	0.829286	-0.343391	-7.284226	0.860549	-0.353718	-7.378423	0.854346	-0.352651	-7.344618
47	Si	0.829928	-4.059205	-6.061886	0.860496	-4.104874	-6.143808	0.854323	-4.085830	-6.115729
48	Si	0.867684	-5.321370	1.888291	0.878652	-5.419335	1.933486	0.874374	-5.385478	1.919876
49	Si	1.977698	8.215165	0.719653	2.021414	8.336219	0.698749	2.007915	8.290731	0.697264
50	Si	1.942322	2.432479	-4.845587	1.972024	2.468788	-4.905654	1.960668	2.453629	-4.881062
51	Si	1.908121	1.113132	3.370314	1.944841	1.138114	3.449055	1.932125	1.130920	3.428304
52	Si	1.997447	-2.604649	4.235763	2.041702	-2.639711	4.324909	2.029792	-2.624605	4.295821
53	Si	1.999472	4.616528	1.855813	2.044067	4.696822	1.907613	2.031889	4.666458	1.893037
54	Si	1.973457	5.376457	4.040870	2.007145	5.428965	4.129191	1.999166	5.404026	4.100404
55	Si	1.666622	1.834567	5.563266	1.711134	1.867438	5.664962	1.695488	1.856621	5.632757
56	Si	1.982974	1.685960	-7.068314	2.038001	1.692252	-7.150930	2.023178	1.685094	-7.116708
57	Si	1.971917	6.064140	-5.884821	1.983387	6.154768	-5.948298	1.974305	6.119996	-5.921011
58	Si	1.919365	-1.271375	-3.853906	1.957429	-1.288558	-3.906523	1.945327	-1.282650	-3.888629
59	Si	1.973576	-1.918959	6.444896	2.008108	-1.910257	6.547134	1.999970	-1.907537	6.509719
60	Si	1.982610	-5.564788	-4.683198	2.037260	-5.616992	-4.746313	2.022377	-5.590578	-4.722176
61	Si	1.940555	-4.841779	-2.452184	1.969722	-4.906474	-2.478824	1.958728	-4.878949	-2.467367
62	Si	1.973862	-6.176096	5.459969	2.017990	-6.286156	5.515343	2.004649	-6.251160	5.487617
63	Si	1.943747	-2.001542	-6.066493	1.994861	-2.025862	-6.142931	1.981692	-2.016336	-6.113707
64	Si	1.968720	-8.376921	-1.130711	1.981455	-8.488759	-1.122524	1.972333	-8.443941	-1.121569
65	Si	3.107289	5.133592	-2.324791	3.147104	5.245967	-2.362046	3.130407	5.209613	-2.348989
66	Si	2.784594	0.239709	6.814412	2.859386	0.259435	6.916563	2.835645	0.256633	6.880310
67	Si	2.783651	3.860980	5.622551	2.858859	3.904438	5.716477	2.835269	3.884734	5.685438
68	Si	3.023321	-2.771061	-2.456422	3.086429	-2.815868	-2.506353	3.067276	-2.798484	-2.491399
69	Si	3.082901	-6.321919	-1.028591	3.129218	-6.414888	-1.037010	3.111959	-6.378993	-1.033653
70	Si	3.102663	-5.510823	1.182059	3.143575	-5.622990	1.218865	3.127241	-5.586156	1.208236
71	Si	3.084481	4.468974	-4.583721	3.131203	4.538694	-4.645719	3.113718	4.511994	-4.622191
72	Si	3.024503	0.764404	-3.617991	3.088208	0.770691	-3.685713	3.068631	0.765906	-3.663897
73	H	-1.771582	9.317623	0.059453	-1.843419	9.430955	0.064330	-1.829555	9.375237	0.062550
74	H	-3.188030	8.168953	-3.075741	-3.201371	8.326923	-3.075530	-3.185783	8.271678	-3.060678
75	H	-1.775197	-7.453293	5.587234	-1.847643	-7.542716	5.658202	-1.833313	-7.499292	5.623943

76	H	-2.487799	1.013095	-9.255805	-2.543488	1.042448	-9.366546	-2.527677	1.036062	-9.317894
77	H	-3.191621	-8.396587	2.385683	-3.205037	-8.523070	2.477543	-3.189060	-8.469907	2.456860
78	H	-2.485931	-6.327444	-6.838745	-2.542443	-6.411513	-6.912002	-2.527048	-6.377540	-6.876305
79	H	-2.368768	-2.672690	-8.110279	-2.418840	-2.702984	-8.202508	-2.402395	-2.689373	-8.161011
80	H	0.003910	8.223261	3.620752	-0.018006	8.331037	3.704868	-0.015390	8.276292	3.685310
81	H	0.001612	-4.457974	7.799462	-0.021839	-4.495698	7.932198	-0.018115	-4.463151	7.883854
82	H	-2.679997	4.557084	-8.276626	-2.694984	4.595430	-8.412955	-2.683525	4.568413	-8.363132
83	H	-0.355748	3.854864	-8.445067	-0.392528	3.877043	-8.546120	-0.393101	3.862211	-8.505388
84	H	-0.358686	-8.129818	-4.493328	-0.395856	-8.203791	-4.564368	-0.396217	-8.167453	-4.540389
85	H	-2.683731	-8.589279	-3.939050	-2.699111	-8.698913	-4.030211	-2.687289	-8.647506	-4.005764
86	H	-0.436727	2.556773	7.763705	-0.457201	2.586537	7.851489	-0.456278	2.573074	7.810075
87	H	-2.515332	6.390624	6.274501	-2.521291	6.489697	6.364905	-2.505864	6.454075	6.338831
88	H	-0.947358	7.356166	-6.050695	-0.940335	7.433895	-6.120257	-0.934731	7.392674	-6.086657
89	H	0.460955	8.298415	-2.839062	0.410542	8.413169	-2.924655	0.412161	8.362473	-2.905248
90	H	-0.949110	-9.514760	-0.487637	-0.943292	-9.617987	-0.499462	-0.937369	-9.564496	-0.496824
91	H	0.456739	-8.357373	2.656227	0.406551	-8.502920	2.651543	0.408499	-8.450179	2.637365
92	H	0.788161	-0.713255	-8.748584	0.837016	-0.720235	-8.842439	0.829355	-0.716471	-8.797462
93	H	0.789761	-4.629960	-7.460267	0.836370	-4.678525	-7.539716	0.829437	-4.655532	-7.500864
94	H	1.277228	9.250631	-0.122929	1.358922	9.337620	-0.208704	1.347541	9.283899	-0.202878
95	H	1.928553	8.678395	2.154547	1.940989	8.877990	2.099297	1.931280	8.821085	2.090795
96	H	1.303656	2.721858	-7.934171	1.384882	2.713889	-8.043548	1.371777	2.700801	-7.998622
97	H	2.683583	7.389013	-5.774810	2.663720	7.490947	-5.817534	2.653266	7.444908	-5.792635
98	H	2.045211	5.622526	-7.324930	2.054214	5.755206	-7.396398	2.040060	5.714414	-7.356487
99	H	1.301556	-6.911468	-4.766102	1.384046	-6.968835	-4.860192	1.370259	-6.931099	-4.829768
100	H	1.920894	-5.701513	6.890971	1.936424	-5.892645	6.964409	1.926616	-5.852535	6.924263
101	H	1.273939	-7.509664	5.390582	1.354767	-7.630168	5.377450	1.343589	-7.584245	5.350773
102	H	2.032736	-8.868764	-2.555019	2.052216	-9.028608	-2.524357	2.037280	-8.970699	-2.517150
103	H	2.683014	-9.384104	-0.265228	2.661069	-9.485707	-0.222775	2.650656	-9.433853	-0.231189
104	H	2.703884	0.549997	8.289551	2.771080	0.569824	8.389058	2.747874	0.564730	8.341609
105	H	2.700261	4.489462	6.992519	2.769087	4.530636	7.084740	2.746494	4.506386	7.043257
106	H	0.519988	-2.537298	0.398482	0.455868	-2.623555	0.445950	0.464530	-2.608405	0.429230
107	H	-0.141143	-0.525632	-1.576190	-0.168975	-0.548275	-1.654516	-0.166276	-0.545599	-1.646655
108	H	0.524717	2.278569	-1.186886	0.457174	2.375020	-1.199866	0.466567	2.353680	-1.204501
109	H	-2.506027	0.428866	1.282023	-2.565897	0.448187	1.346119	-2.549305	0.444436	1.337993
110	H	0.616433	1.982991	0.659393	0.667989	2.028443	0.731196	0.657138	2.010089	0.728437
111	H	0.620394	-1.198985	1.705053	0.669258	-1.193984	1.791417	0.658228	-1.181762	1.779064
112	H	-3.117493	2.306477	-0.909199	-3.146190	2.412649	-0.943051	-3.128052	2.391977	-0.929110
113	H	-3.120786	-2.396411	0.637251	-3.148225	-2.500704	0.673624	-3.130467	-2.475889	0.673531
114	H	2.953751	1.082030	-2.143563	3.036924	1.079543	-2.215119	3.011804	1.067668	-2.204242
115	H	2.952991	-2.154071	-1.080283	3.034176	-2.192719	-1.139101	3.010534	-2.175761	-1.137278
116	H	-0.107718	6.300021	6.362047	-0.133832	6.375684	6.450890	-0.129868	6.337021	6.406774
117	H	-2.517506	-1.404635	8.840326	-2.522591	-1.430963	8.973482	-2.507508	-1.418515	8.931605
118	H	0.503192	5.649103	4.247023	0.533464	5.614865	4.354056	0.540110	5.608292	4.312718
119	H	2.677081	-2.914055	7.336060	2.634175	-2.903532	7.484540	2.644921	-2.891265	7.427627
120	H	-2.423729	-4.543942	7.932825	-2.429404	-4.581547	8.060943	-2.411199	-4.561003	8.015544
121	H	-2.421564	8.372970	3.676161	-2.425574	8.479607	3.756543	-2.408445	8.434968	3.732122
122	H	0.504772	-2.020854	6.777824	0.535655	-1.930276	6.844283	0.542218	-1.949709	6.807533
123	H	-0.110477	-1.279608	8.859591	-0.135442	-1.288222	8.976333	-0.131794	-1.283892	8.918617

124	H	2.672447	6.708419	4.170958	2.627552	6.786964	4.297462	2.638908	6.742783	4.257898
125	Tv	6.669314	0.003423	0.011035	6.795620	0.006929	0.023008	6.754540	0.006843	0.022954

	Atomic Type	SiNW [112] - LDA			SiNW [112] - GGA			SiNW [112] - HSE		
1	Si	-2.531062	8.024346	-0.001373	-2.573435	8.118029	0.935750	-2.557145	8.075776	-0.000612
2	Si	-2.526648	7.307119	-2.231334	-2.575810	7.361337	-2.335921	-2.547210	7.346680	-2.240593
3	Si	-2.509452	4.412520	1.138299	-2.548388	4.488967	1.102592	-2.535421	4.450875	1.150288
4	Si	-2.547278	0.809251	2.442986	-2.589603	0.843278	2.451084	-2.578867	0.812774	2.454812
5	Si	-2.522970	3.680425	-1.082997	-2.578204	3.718164	-1.139419	-2.550183	3.707737	-1.087344
6	Si	-2.512046	-2.860657	3.544621	-2.546084	-2.863759	3.617866	-2.537538	-2.885215	3.577074
7	Si	-2.545700	0.063879	0.195077	-2.599207	0.066072	0.181871	-2.573532	0.062666	0.190193
8	Si	-2.534565	-6.439954	4.784548	-2.567855	-6.466126	4.894306	-2.559919	-6.481932	4.814492
9	Si	-2.524481	-3.600290	1.325780	-2.575274	-3.629090	1.374029	-2.551557	-3.624559	1.338175
10	Si	-2.523978	1.475251	-7.735452	-2.624371	1.400687	-7.846794	-2.553143	1.471698	-7.784570
11	Si	-2.528934	-7.195919	2.567588	-2.569154	-7.242056	2.658704	-2.549200	-7.233416	2.582072
12	Si	-2.523788	-5.800824	-5.327985	-2.620631	-5.907094	-5.347480	-2.553647	-5.825127	-5.370942
13	Si	-2.544425	-2.155609	-6.510412	-2.639702	-2.243114	-6.567256	-2.570124	-2.167344	-6.549272
14	Si	-1.324675	7.375249	3.530009	-1.314317	7.502805	3.494587	-1.328648	7.428611	3.571260
15	Si	-1.410412	6.473196	1.353375	-1.420191	6.576499	1.293628	-1.418582	6.527075	1.370939
16	Si	-1.644154	3.631650	4.824356	-1.646370	3.720624	4.837697	-1.659552	3.652658	4.863435
17	Si	-1.643695	-0.039219	6.038662	-1.644180	0.031066	6.100645	-1.659521	-0.032109	6.082428
18	Si	-1.432534	4.283859	-5.385687	-1.509990	4.277850	-5.522654	-1.461042	4.310774	-5.434056
19	Si	-1.450566	2.898008	2.576174	-1.467485	2.959501	2.560527	-1.466620	2.918002	2.591710
20	Si	-1.450766	-0.788251	3.795600	-1.465378	-0.761323	3.833996	-1.466902	-0.795831	3.820307
21	Si	-1.324721	-3.816220	7.231229	-1.311914	-3.781732	7.354694	-1.329890	-3.834123	7.296313
22	Si	-1.438466	0.637180	-4.173578	-1.500892	0.604006	-4.242304	-1.455478	0.643420	-4.198314
23	Si	-1.439046	-3.000671	-2.970068	-1.499301	-3.066749	-2.986668	-1.456105	-3.020005	-2.986493
24	Si	-1.413039	-4.387147	4.945428	-1.416658	-4.396790	5.046892	-1.421061	-4.420995	4.991874
25	Si	-1.433901	-6.650661	-1.766240	-1.505141	-6.754898	-1.747878	-1.462438	-6.700717	-1.790640
26	Si	-1.424148	-0.098018	-6.400420	-1.491065	-0.167451	-6.487514	-1.432264	-0.100718	-6.439625
27	Si	-1.663337	3.647458	-7.624195	-1.755378	3.597410	-7.778584	-1.692045	3.658894	-7.688071
28	Si	-1.424033	-3.741677	-5.194920	-1.489082	-3.834016	-5.233287	-1.432422	-3.761093	-5.228760
29	Si	-1.665750	-7.477330	-3.941197	-1.751957	-7.600332	-3.946825	-1.694626	-7.522809	-3.987842
30	Si	-0.522629	2.021457	6.112482	-0.486581	2.106269	6.140239	-0.513856	2.035172	6.152966
31	Si	-1.341614	5.910093	5.374769	-1.329120	6.035210	5.371419	-1.354628	5.950147	5.425507
32	Si	-0.317286	3.438317	-1.845048	-0.343791	3.460717	-1.921980	-0.323125	3.462941	-1.854185
33	Si	-0.308656	6.333055	-5.240617	-0.356330	6.342605	-5.388886	-0.319561	6.367049	-5.273899
34	Si	-0.333996	7.067912	-3.022345	-0.370051	7.102199	-3.153071	-0.345856	7.100936	-3.041295
35	Si	-0.343037	-0.198877	-0.604437	-0.363563	-0.207827	-0.626750	-0.345554	-0.199024	-0.603937
36	Si	-1.342511	-1.540099	7.839307	-1.327647	-1.472075	7.940147	-1.355815	-1.541489	7.903685
37	Si	-0.318523	-3.858299	0.569486	-0.340685	-3.900943	0.596673	-0.324324	-3.884100	0.576520
38	Si	-0.313009	2.695725	-4.067697	-0.357558	2.689938	-4.169272	-0.321954	2.718707	-4.097028
39	Si	-0.327649	-0.936828	-2.831143	-0.363574	-0.977512	-2.873843	-0.330674	-0.941744	-2.846535
40	Si	-0.314305	-4.589956	-1.656750	-0.354495	-4.669870	-1.651328	-0.323229	-4.625636	-1.667161
41	Si	-0.310820	-8.209164	-0.427270	-0.349552	-8.304434	-0.378416	-0.321351	-8.256356	-0.436091
42	Si	-0.335730	-7.473978	1.790840	-0.363020	-7.533900	1.853635	-0.347534	-7.512683	1.793238
43	Si	0.782711	6.229598	0.540266	0.800125	6.317347	0.457049	0.795172	6.281434	0.549440
44	Si	0.784923	5.506168	-1.685953	0.787407	5.549997	-1.787704	0.797139	5.541972	-1.691838

45	Si	0.764185	1.866680	-0.475826	0.767391	1.882440	-0.529150	0.775540	1.880229	-0.478689
46	Si	0.763579	-1.780533	0.730578	0.768972	-1.799475	0.730222	0.774937	-1.793723	0.736598
47	Si	0.751073	-1.040879	2.957499	0.770784	-1.032615	2.979914	0.761502	-1.053079	2.981343
48	Si	0.751516	2.604318	1.752063	0.768942	2.656189	1.718175	0.761979	2.626375	1.764385
49	Si	0.780341	-4.673742	4.147631	0.804088	-4.699123	4.225999	0.792878	-4.711791	4.185805
50	Si	0.793729	-0.342422	-7.106527	0.753455	-0.427464	-7.209070	0.804540	-0.349704	-7.149324
51	Si	0.793699	-3.965782	-5.908157	0.755243	-4.067607	-5.964370	0.804241	-3.984241	-5.947346
52	Si	0.783580	-5.423514	1.930416	0.792239	-5.469366	1.982250	0.795646	-5.456648	1.946493
53	Si	1.931973	8.255676	0.737059	1.968473	8.375151	0.570023	1.952622	8.330292	0.692063
54	Si	1.917428	2.448925	-4.765177	1.905357	2.430140	-4.884233	1.932614	2.470856	-4.797774
55	Si	1.852747	1.018921	3.072871	1.891323	1.056593	3.063241	1.872359	1.024611	3.093124
56	Si	1.931000	-2.640703	4.193430	1.980110	-2.641582	4.244142	1.958779	-2.663688	4.229371
57	Si	1.933718	4.624768	1.788979	1.977959	4.703164	1.731217	1.961075	4.662902	1.805311
58	Si	1.946105	5.361355	3.973239	1.989367	5.431750	3.943884	1.968190	5.373920	4.010840
59	Si	1.634486	1.745022	5.276221	1.696049	1.816177	5.286371	1.662170	1.756605	5.310924
60	Si	1.945768	1.685839	-6.979234	1.938846	1.610948	-7.109170	1.977240	1.681504	-7.020661
61	Si	1.889959	6.038434	-5.982080	1.877135	6.087725	-6.116532	1.907092	6.120857	-5.990312
62	Si	1.900586	-1.177303	-3.556210	1.895962	-1.230476	-3.615847	1.920759	-1.182888	-3.573954
63	Si	1.947349	-1.934796	6.387189	1.993059	-1.863391	6.439375	1.968610	-1.922560	6.424601
64	Si	1.945221	-5.518881	-4.596907	1.942199	-5.617357	-4.638008	1.976423	-5.538672	-4.633094
65	Si	1.915849	-4.810292	-2.364272	1.908132	-4.902156	-2.376962	1.931121	-4.846470	-2.377679
66	Si	1.927717	-6.184801	5.513327	1.973556	-6.257552	5.573275	1.949361	-6.273060	5.520965
67	Si	1.909413	-1.914892	-5.783638	1.897417	-1.999788	-5.863599	1.936095	-1.925506	-5.817600
68	Si	1.885747	-8.415619	-1.203759	1.883131	-8.547639	-1.112349	1.904237	-8.487047	-1.160859
69	Si	3.011651	5.260555	-2.400825	3.041834	5.290975	-2.523700	3.043739	5.294544	-2.414289
70	Si	2.772775	0.230572	6.602919	2.865916	0.308074	6.630897	2.819176	0.244194	6.641482
71	Si	2.771988	3.751889	5.437871	2.863445	3.833039	5.425230	2.818886	3.763946	5.477154
72	Si	3.007597	1.624194	-1.171469	3.042047	1.628785	-1.242207	3.041752	1.638174	-1.177531
73	Si	3.006768	-2.003047	0.027467	3.043491	-2.035120	0.010227	3.041014	-2.017887	0.031246
74	Si	3.016197	-2.741863	-2.207780	3.036677	-2.808356	-2.245277	3.049158	-2.763782	-2.219559
75	Si	3.024410	-6.381099	-1.017194	3.042367	-6.482944	-1.005600	3.053108	-6.431656	-1.023314
76	Si	3.010001	-5.654289	1.210596	3.046457	-5.713949	1.241156	3.042070	-5.689993	1.219400
77	Si	3.026024	4.512471	-4.621594	3.037503	4.520172	-4.769885	3.054593	4.550408	-4.656209
78	Si	3.017267	0.882024	-3.405640	3.035541	0.856752	-3.498081	3.050096	0.893169	-3.428651
79	H	-1.816033	9.352754	0.092543	-1.877216	9.455975	-0.030919	-1.866555	9.402775	0.080395
80	H	-3.261516	8.320484	-3.080146	-3.290228	8.384210	-3.185622	-3.254973	8.367969	-3.077719
81	H	-1.820728	-7.449899	5.653642	-1.871623	-7.484344	5.764495	-1.870668	-7.498676	5.672173
82	H	-2.539709	0.980291	-9.162370	-2.651419	0.892384	-9.267608	-2.570971	0.980536	-9.199390
83	H	-3.263810	-8.515397	2.489108	-3.282587	-8.571490	2.612598	-3.257127	-8.552270	2.518058
84	H	-2.538610	-6.254513	-6.768587	-2.647037	-6.375226	-6.782060	-2.571044	-6.274526	-6.799586
85	H	-2.561940	-2.629637	-7.945877	-2.665814	-2.731156	-7.996043	-2.586326	-2.637501	-7.972073
86	H	-0.050473	8.183018	3.577607	-0.044485	8.308736	3.541796	-0.066608	8.225858	3.633715
87	H	-0.050062	-4.436797	7.749168	-0.042235	-4.389280	7.886657	-0.067857	-4.437182	7.821408
88	H	-2.706028	4.559845	-8.223723	-2.780154	4.502525	-8.408621	-2.714334	4.560001	-8.301961
89	H	-0.389535	3.833596	-8.404370	-0.488278	3.756379	-8.567933	-0.432427	3.831456	-8.465134
90	H	-0.393275	-8.095413	-4.455834	-0.485586	-8.211201	-4.473136	-0.436162	-8.127361	-4.508409
91	H	-2.710674	-8.565074	-3.876407	-2.777669	-8.700758	-3.888385	-2.718676	-8.610551	-3.941453
92	H	-0.385020	2.494083	7.540690	-0.347640	2.593125	7.561659	-0.384007	2.503772	7.569141

93	H	-2.588928	6.232112	6.170103	-2.553482	6.388377	6.181247	-2.571318	6.266234	6.232418
94	H	-1.025797	7.330355	-6.120986	-1.054576	7.350041	-6.269525	-1.010484	7.373397	-6.141938
95	H	0.390482	8.389961	-2.905192	0.334900	8.434482	-3.077133	0.353289	8.422287	-2.946646
96	H	-2.590658	-1.324565	8.668631	-2.551279	-1.254416	8.797465	-2.572986	-1.330170	8.751225
97	H	-1.029763	-9.533726	-0.538912	-1.048044	-9.640085	-0.456206	-1.013914	-9.580985	-0.532200
98	H	0.388307	-8.464952	2.674207	0.342763	-8.540099	2.729557	0.351118	-8.517105	2.657436
99	H	0.795069	-0.832498	-8.536393	0.744298	-0.928490	-8.633325	0.804993	-0.832860	-8.567619
100	H	0.794812	-4.423713	-7.348672	0.745890	-4.542682	-7.397517	0.804516	-4.441442	-7.374236
101	H	1.220925	9.318725	-0.061097	1.292097	9.385399	-0.317110	1.282549	9.339825	-0.182337
102	H	1.922650	8.680891	2.184243	1.925498	8.909768	1.974691	1.903852	8.840175	2.094184
103	H	1.252594	2.725929	-7.829548	1.269110	2.629809	-7.992602	1.313425	2.701939	-7.887818
104	H	2.627237	7.353451	-5.988574	2.575962	7.419164	-6.052897	2.601369	7.441617	-5.910646
105	H	1.868953	5.515808	-7.396532	1.889611	5.641713	-7.552370	1.923478	5.684605	-7.417842
106	H	1.250793	-6.860132	-4.661423	1.273029	-6.964031	-4.713928	1.311921	-6.874502	-4.722158
107	H	1.915827	-5.667318	6.930076	1.929557	-5.823246	7.012015	1.899554	-5.848873	6.951248
108	H	1.215995	-7.513804	5.500961	1.297169	-7.599303	5.487051	1.278113	-7.604122	5.417924
109	H	1.857791	-8.831256	-2.653306	1.893364	-9.070743	-2.522048	1.917096	-8.983302	-2.568805
110	H	2.623478	-9.481490	-0.434148	2.582714	-9.563784	-0.250332	2.598519	-9.503819	-0.314212
111	H	2.715784	0.671563	8.046088	2.802809	0.764107	8.066832	2.750105	0.683681	8.070279
112	H	2.714117	4.259331	6.859055	2.800258	4.351704	6.839781	2.749379	4.263495	6.886082
113	H	-3.995634	6.678903	4.098805	-4.142477	6.786986	4.127749	-4.101524	6.695997	4.157250
114	H	4.194547	8.343679	3.660418	4.333820	8.472641	3.598836	4.286240	8.397607	3.714662
115	H	-0.187635	6.173030	6.303525	-0.168345	6.301309	6.286970	-0.199470	6.201289	6.334180
116	H	0.492730	-2.036478	6.767932	0.532355	-1.873870	6.780296	0.524712	-1.966803	6.771693
117	H	-3.988566	-2.920044	7.265782	-4.137157	-2.830129	7.414523	-4.098205	-2.897756	7.325811
118	H	4.195370	-4.517176	7.913547	4.336319	-4.478432	8.028042	4.285058	-4.527512	7.989353
119	H	-0.189875	-1.196351	8.742889	-0.166901	-1.121484	8.826796	-0.201464	-1.201033	8.783791
120	H	0.489086	5.660898	4.215502	0.528338	5.647073	4.207489	0.523127	5.611703	4.261205
121	Tv	6.669260	-0.000882	-0.002569	6.782724	-0.009309	-0.038596	6.744062	0.000133	0.001681