

# Supporting Information for: Gas separation through bilayer silica, the thinnest possible silica membrane

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Optimized Crystalline bilayer silica

1.0

21.189300000	0.000000000	0.000000000
10.594600000	18.350400000	0.000000000
0.000000000	0.000000000	15.000000000

Si 0

64 128

Cartesian

0.000000	-0.000040	7.000760
2.648658	4.587570	7.000760
5.297316	9.175179	7.000760
7.945975	13.762790	7.000760
5.297316	-0.000040	7.000760
7.945974	4.587570	7.000760
10.594632	9.175179	7.000760
13.243291	13.762790	7.000760
10.594631	-0.000040	7.000760
13.243289	4.587570	7.000760
15.891947	9.175179	7.000760
18.540606	13.762790	7.000760
15.891947	-0.000040	7.000760
18.540604	4.587570	7.000760
21.189262	9.175179	7.000760
23.837921	13.762790	7.000760
2.648660	1.529200	7.001090
5.297318	6.116810	7.001090
7.945976	10.704419	7.001090
10.594634	15.292028	7.001090
7.945976	1.529200	7.001090
10.594634	6.116810	7.001090
13.243292	10.704419	7.001090
15.891950	15.292028	7.001090
13.243291	1.529200	7.001090
15.891949	6.116810	7.001090
18.540607	10.704419	7.001090
21.189264	15.292028	7.001090
18.540606	1.529200	7.001090
21.189264	6.116810	7.001090
23.837923	10.704419	7.001090
26.486580	15.292028	7.001090
0.000000	-0.000040	3.751960
2.648658	4.587570	3.751960
5.297316	9.175179	3.751960
7.945975	13.762790	3.751960
5.297316	-0.000040	3.751960
7.945974	4.587570	3.751960
10.594632	9.175179	3.751960
13.243291	13.762790	3.751960
10.594631	-0.000040	3.751960
13.243289	4.587570	3.751960

15.891947	9.175179	3.751960
18.540606	13.762790	3.751960
15.891947	-0.000040	3.751960
18.540604	4.587570	3.751960
21.189262	9.175179	3.751960
23.837921	13.762790	3.751960
2.648660	1.529200	3.751630
5.297318	6.116810	3.751630
7.945976	10.704419	3.751630
10.594634	15.292028	3.751630
7.945976	1.529200	3.751630
10.594634	6.116810	3.751630
13.243292	10.704419	3.751630
15.891950	15.292028	3.751630
13.243291	1.529200	3.751630
15.891949	6.116810	3.751630
18.540607	10.704419	3.751630
21.189264	15.292028	3.751630
18.540606	1.529200	3.751630
21.189264	6.116810	3.751630
23.837923	10.704419	3.751630
26.486580	15.292028	3.751630
1.324170	0.764480	7.549560
3.972828	5.352090	7.549560
6.621487	9.939700	7.549560
9.270144	14.527309	7.549560
6.621486	0.764480	7.549560
9.270144	5.352090	7.549560
11.918802	9.939700	7.549560
14.567460	14.527309	7.549560
11.918800	0.764480	7.549560
14.567459	5.352090	7.549560
17.216118	9.939700	7.549560
19.864775	14.527309	7.549560
17.216116	0.764480	7.549560
19.864775	5.352090	7.549560
22.513433	9.939700	7.549560
25.162090	14.527309	7.549560
3.973140	0.764480	7.549560
6.621799	5.352090	7.549560
9.270456	9.939700	7.549560
11.919115	14.527309	7.549560
9.270456	0.764480	7.549560
11.919114	5.352090	7.549560
14.567773	9.939700	7.549560
17.216431	14.527309	7.549560
14.567772	0.764480	7.549560
17.216431	5.352090	7.549560
19.865088	9.939700	7.549560
22.513746	14.527309	7.549560

19.865088	0.764480	7.549560
22.513746	5.352090	7.549560
25.162403	9.939700	7.549560
27.811062	14.527309	7.549560
2.648660	3.058520	7.549541
5.297318	7.646130	7.549541
7.945976	12.233739	7.549541
10.594634	16.821348	7.549541
7.945976	3.058520	7.549541
10.594634	7.646130	7.549541
13.243292	12.233739	7.549541
15.891950	16.821348	7.549541
13.243291	3.058520	7.549541
15.891949	7.646130	7.549541
18.540607	12.233739	7.549541
21.189264	16.821348	7.549541
18.540606	3.058520	7.549541
21.189264	7.646130	7.549541
23.837923	12.233739	7.549541
26.486580	16.821348	7.549541
1.324170	0.764480	3.203160
3.972828	5.352090	3.203160
6.621487	9.939700	3.203160
9.270144	14.527309	3.203160
6.621486	0.764480	3.203160
9.270144	5.352090	3.203160
11.918802	9.939700	3.203160
14.567460	14.527309	3.203160
11.918800	0.764480	3.203160
14.567459	5.352090	3.203160
17.216118	9.939700	3.203160
19.864775	14.527309	3.203160
17.216116	0.764480	3.203160
19.864775	5.352090	3.203160
22.513433	9.939700	3.203160
25.162090	14.527309	3.203160
3.973140	0.764480	3.203160
6.621799	5.352090	3.203160
9.270456	9.939700	3.203160
11.919115	14.527309	3.203160
9.270456	0.764480	3.203160
11.919114	5.352090	3.203160
14.567773	9.939700	3.203160
17.216431	14.527309	3.203160
14.567772	0.764480	3.203160
17.216431	5.352090	3.203160
19.865088	9.939700	3.203160
22.513746	14.527309	3.203160
19.865088	0.764480	3.203160
22.513746	5.352090	3.203160

25.162403	9.939700	3.203160
27.811062	14.527309	3.203160
2.648660	3.058520	3.203180
5.297318	7.646130	3.203180
7.945976	12.233739	3.203180
10.594634	16.821348	3.203180
7.945976	3.058520	3.203180
10.594634	7.646130	3.203180
13.243292	12.233739	3.203180
15.891950	16.821348	3.203180
13.243291	3.058520	3.203180
15.891949	7.646130	3.203180
18.540607	12.233739	3.203180
21.189264	16.821348	3.203180
18.540606	3.058520	3.203180
21.189264	7.646130	3.203180
23.837923	12.233739	3.203180
26.486580	16.821348	3.203180
-0.000000	-0.000030	5.376360
2.648658	4.587580	5.376360
5.297316	9.175189	5.376360
7.945974	13.762798	5.376360
5.297315	-0.000030	5.376360
7.945973	4.587580	5.376360
10.594631	9.175189	5.376360
13.243289	13.762798	5.376360
10.594631	-0.000030	5.376360
13.243290	4.587580	5.376360
15.891948	9.175189	5.376360
18.540606	13.762798	5.376360
15.891947	-0.000030	5.376360
18.540606	4.587580	5.376360
21.189262	9.175189	5.376360
23.837921	13.762798	5.376360
2.648660	1.529180	5.376360
5.297318	6.116790	5.376360
7.945976	10.704399	5.376360
10.594634	15.292009	5.376360
7.945975	1.529180	5.376360
10.594633	6.116790	5.376360
13.243292	10.704399	5.376360
15.891950	15.292009	5.376360
13.243292	1.529180	5.376360
15.891950	6.116790	5.376360
18.540607	10.704399	5.376360
21.189266	15.292009	5.376360
18.540607	1.529180	5.376360
21.189266	6.116790	5.376360
23.837923	10.704399	5.376360
26.486582	15.292009	5.376360

Optimized Stone-Wales defect

1

21.100464	0	0.0000000000	
10.550232	18.273618	0.0000000000	
0.0000000000	0.0000000000		15.0000000000

Si 0

64 128

Cartesian

2.48228	1.43248	0.99777
5.13792	2.96569	1.00063
4.93579	6.03968	0.99757
7.47759	7.83092	1.00264
7.10488	10.83200	1.00005
9.69018	12.36872	1.00057
9.97503	15.31253	1.00296
12.63621	16.68479	0.99878
7.69956	1.25430	0.99763
10.52181	2.56049	1.00271
10.49633	7.76534	1.00039
11.97305	5.20850	1.00039
11.99102	10.43847	0.99979
14.81906	11.71526	0.99782
15.06538	14.82664	0.99954
17.72515	16.44784	0.99957
12.93432	0.73669	1.00017
15.55658	2.20838	1.00054
15.03521	5.16552	0.99976
17.55572	6.97552	0.99781
17.41616	10.05493	1.00020
20.07122	11.58783	0.99875
20.21573	14.64792	0.99873
22.89726	16.08447	1.00007
18.24779	0.98417	1.00296
20.76796	2.59997	0.99879
20.37314	5.63298	0.99950
23.10679	7.12601	0.99956
22.79352	10.18275	0.99871
25.37777	11.78771	1.00009
25.62303	14.79369	0.99967
28.25019	16.31176	0.99826
2.48228	1.43248	4.24982
5.13792	2.96569	4.24696
4.93579	6.03968	4.25002
7.47759	7.83092	4.24495
7.10488	10.83200	4.24754
9.69018	12.36872	4.24702
9.97503	15.31253	4.24463
12.63621	16.68479	4.24881
7.69956	1.25430	4.24996
10.52181	2.56049	4.24488

10.49633	7.76534	4.24720
11.97305	5.20850	4.24720
11.99102	10.43847	4.24780
14.81906	11.71526	4.24977
15.06538	14.82664	4.24805
17.72515	16.44784	4.24802
12.93432	0.73669	4.24742
15.55658	2.20838	4.24705
15.03521	5.16552	4.24783
17.55572	6.97552	4.24978
17.41616	10.05493	4.24739
20.07122	11.58783	4.24884
20.21573	14.64792	4.24886
22.89726	16.08447	4.24752
18.24779	0.98417	4.24463
20.76796	2.59997	4.24880
20.37314	5.63298	4.24809
23.10679	7.12601	4.24803
22.79352	10.18275	4.24888
25.37777	11.78771	4.24750
25.62303	14.79369	4.24792
28.25019	16.31176	4.24933
3.80828	2.19788	0.44553
5.14672	4.50800	0.47472
6.47832	2.20271	0.47480
6.20722	6.94039	0.45040
7.43286	9.35335	0.45615
8.97207	7.41576	0.49453
8.20353	11.92458	0.46204
10.22278	13.80561	0.48432
10.84035	11.41049	0.42444
11.14417	16.30014	0.44747
13.71318	15.57941	0.47887
13.03570	18.16703	0.45651
9.11565	1.90516	0.45051
10.90871	4.06256	0.49436
11.81867	1.76155	0.45651
11.31546	6.53351	0.41390
11.42578	9.00469	0.47014
13.51113	5.39549	0.47064
13.45263	10.96554	0.46305
15.00600	13.26854	0.47323
16.08856	10.83623	0.46841
16.35366	15.70761	0.47230
18.97683	15.55260	0.46666
17.95293	17.99186	0.47661
14.43023	1.14087	0.46220
15.29835	3.68273	0.42382
17.06840	1.95496	0.48546
16.22333	6.16686	0.46299

17.42946	8.51438	0.46851
18.99424	6.36029	0.47311
18.74533	10.82263	0.45225
20.06570	13.12284	0.45423
21.39751	10.81501	0.45424
21.60937	15.27667	0.43390
24.27707	15.47269	0.43851
22.92498	17.59971	0.44403
19.68858	1.50037	0.44726
20.34944	4.08557	0.47902
22.25134	2.20473	0.45642
21.77996	6.30856	0.47218
22.95793	8.65757	0.46659
24.55760	6.55070	0.47655
24.03454	11.07583	0.43396
25.53709	13.28856	0.43844
26.70410	11.05454	0.44414
26.93839	15.55285	0.42070
29.59998	15.63317	0.43160
28.33361	17.82065	0.43235
3.80828	2.19788	4.80206
5.14672	4.50800	4.77287
6.47832	2.20271	4.77279
6.20722	6.94039	4.79719
7.43286	9.35335	4.79144
8.97207	7.41576	4.75306
8.20353	11.92458	4.78555
10.22278	13.80561	4.76327
10.84035	11.41049	4.82315
11.14417	16.30014	4.80012
13.71318	15.57941	4.76872
13.03570	18.16703	4.79108
9.11565	1.90516	4.79708
10.90871	4.06256	4.75323
11.81867	1.76155	4.79108
11.31546	6.53351	4.83369
11.42578	9.00469	4.77745
13.51113	5.39549	4.77695
13.45263	10.96554	4.78454
15.00600	13.26854	4.77436
16.08856	10.83623	4.77918
16.35366	15.70761	4.77529
18.97683	15.55260	4.78093
17.95293	17.99186	4.77098
14.43023	1.14087	4.78539
15.29835	3.68273	4.82377
17.06840	1.95496	4.76213
16.22333	6.16686	4.78460
17.42946	8.51438	4.77908
18.99424	6.36029	4.77448

18.74533	10.82263	4.79534
20.06570	13.12284	4.79336
21.39751	10.81501	4.79335
21.60937	15.27667	4.81369
24.27707	15.47269	4.80908
22.92498	17.59971	4.80356
19.68858	1.50037	4.80033
20.34944	4.08557	4.76857
22.25134	2.20473	4.79117
21.77996	6.30856	4.77541
22.95793	8.65757	4.78100
24.55760	6.55070	4.77104
24.03454	11.07583	4.81363
25.53709	13.28856	4.80915
26.70410	11.05454	4.80345
26.93839	15.55285	4.82689
29.59998	15.63317	4.81599
28.33361	17.82065	4.81524
2.48361	1.43345	2.62380
5.11365	2.95166	2.62380
4.93741	6.08043	2.62380
7.40042	7.77785	2.62380
7.11171	10.87241	2.62380
9.64941	12.33692	2.62380
9.96688	15.39720	2.62380
12.62930	16.69379	2.62380
7.73584	1.23531	2.62380
10.43706	2.52042	2.62380
10.44379	7.86717	2.62380
12.03466	5.11191	2.62380
12.05799	10.43894	2.62380
14.79600	11.74136	2.62380
15.10862	14.80586	2.62380
17.69323	16.47399	2.62380
12.97270	0.72199	2.62380
15.50819	2.18934	2.62380
15.06981	5.22296	2.62380
17.56665	6.94252	2.62380
17.42466	10.05985	2.62380
20.07891	11.59234	2.62380
20.22739	14.64852	2.62380
22.86501	16.05050	2.62380
18.31819	0.93447	2.62380
20.77242	2.58939	2.62380
20.37669	5.68094	2.62380
23.11342	7.08541	2.62380
22.79967	10.19261	2.62380
25.33227	11.77678	2.62380
25.66267	14.81650	2.62380
28.20851	16.28704	2.62380

Optimized 555777 Defect

1.0

20.961300000	0.0000000000	0.0000000000
10.480600000	18.153000000	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Si 0

60 120

Cartesian

1.96881	1.65376	0.99812
4.80519	2.77488	1.00153
5.24364	5.79347	0.99849
7.98905	7.27834	0.99942
7.98566	10.37737	0.99960
10.55122	12.14642	0.99908
9.82689	15.17631	1.00189
12.47428	16.70479	1.00190
7.18256	0.86588	0.99815
9.84497	2.46463	1.00135
10.54627	5.49861	0.99946
13.65975	6.01939	0.99978
13.65538	11.59895	1.00007
15.26773	8.81007	0.99909
14.73554	14.56138	0.99922
17.55033	15.89846	0.99961
12.49545	0.93327	1.00142
14.76669	3.06521	0.99926
18.48873	8.80737	0.99981
20.49642	11.24187	0.99940
20.23371	14.34713	0.99952
22.89306	15.98324	0.99848
17.57249	1.71774	0.99961
20.25729	3.26722	0.99949
20.49364	6.37088	0.99940
23.47545	7.27091	1.00147
23.47419	10.33246	1.00141
26.18849	11.84079	0.99819
25.72555	14.85379	1.00134
28.11472	16.74980	0.99812
1.96881	1.65376	4.24947
4.80519	2.77488	4.24606
5.24364	5.79347	4.24910
7.98905	7.27834	4.24817
7.98566	10.37737	4.24799
10.55122	12.14642	4.24851
9.82689	15.17631	4.24570
12.47428	16.70479	4.24569
7.18256	0.86588	4.24944
9.84497	2.46463	4.24624
10.54627	5.49861	4.24813
13.65975	6.01939	4.24781

13.65538	11.59895	4.24752
15.26773	8.81007	4.24850
14.73554	14.56138	4.24837
17.55033	15.89846	4.24798
12.49545	0.93327	4.24617
14.76669	3.06521	4.24833
18.48873	8.80737	4.24778
20.49642	11.24187	4.24819
20.23371	14.34713	4.24807
22.89306	15.98324	4.24911
17.57249	1.71774	4.24798
20.25729	3.26722	4.24810
20.49364	6.37088	4.24819
23.47545	7.27091	4.24612
23.47419	10.33246	4.24618
26.18849	11.84079	4.24940
25.72555	14.85379	4.24625
28.11472	16.74980	4.24947
3.28852	2.46821	0.47753
5.29857	4.24243	0.48110
5.82763	1.61640	0.47290
6.59912	6.56407	0.46914
8.01660	8.82794	0.47564
9.36542	6.52796	0.48985
9.35768	11.13281	0.48841
10.13735	13.65178	0.46759
12.06443	11.66517	0.50407
11.03334	16.14372	0.49835
13.63959	15.67369	0.46813
2.10411	0.10064	0.46675
8.46787	1.74714	0.46719
10.10861	3.99896	0.47129
11.07841	1.54004	0.48754
12.06774	5.95559	0.50510
14.46168	7.41305	0.51346
14.39976	4.60963	0.50122
14.46037	10.20692	0.51356
14.39345	13.01046	0.50492
16.88063	8.80987	0.51346
16.21046	15.08711	0.48826
18.87757	15.09778	0.47602
17.63033	17.45948	0.47136
13.69108	1.93090	0.47275
16.24902	2.55832	0.49087
19.33997	10.15345	0.50400
19.33908	7.46088	0.50212
20.19599	12.77964	0.49055
22.01363	10.87056	0.47096
21.54790	15.19359	0.47022
24.20863	15.16117	0.47973

23.04178	17.53461	0.46602
18.91637	2.48996	0.47529
20.19080	4.83384	0.49108
21.58786	2.44792	0.46988
22.01337	6.73552	0.47195
23.65987	8.80191	0.48860
3.82493	6.43832	0.46584
24.78291	11.16793	0.46697
26.21730	13.38910	0.47244
6.59371	11.08854	0.47196
26.74978	16.01359	0.47784
29.39200	15.85573	0.46697
17.61732	0.15594	0.46982
3.28852	2.46821	4.77006
5.29857	4.24243	4.76649
5.82763	1.61640	4.77469
6.59912	6.56407	4.77845
8.01660	8.82794	4.77195
9.36542	6.52796	4.75774
9.35768	11.13281	4.75918
10.13735	13.65178	4.78000
12.06443	11.66517	4.74352
11.03334	16.14372	4.74925
13.63959	15.67369	4.77946
2.10411	0.10064	4.78084
8.46787	1.74714	4.78040
10.10861	3.99896	4.77630
11.07841	1.54004	4.76005
12.06774	5.95559	4.74249
14.46168	7.41305	4.73413
14.39976	4.60963	4.74637
14.46037	10.20692	4.73403
14.39345	13.01046	4.74267
16.88063	8.80987	4.73413
16.21046	15.08711	4.75933
18.87757	15.09778	4.77157
17.63033	17.45948	4.77623
13.69108	1.93090	4.77484
16.24902	2.55832	4.75672
19.33997	10.15345	4.74359
19.33908	7.46088	4.74547
20.19599	12.77964	4.75704
22.01363	10.87056	4.77663
21.54790	15.19359	4.77737
24.20863	15.16117	4.76786
23.04178	17.53461	4.78157
18.91637	2.48996	4.77231
20.19080	4.83384	4.75651
21.58786	2.44792	4.77771
22.01337	6.73552	4.77564

23.65987	8.80191	4.75899
3.82493	6.43832	4.78175
24.78291	11.16793	4.78062
26.21730	13.38910	4.77515
6.59371	11.08854	4.77563
26.74978	16.01359	4.76975
29.39200	15.85573	4.78062
17.61732	0.15594	4.77777
1.93104	1.63357	2.62380
4.80799	2.77113	2.62380
5.24389	5.84413	2.62380
7.97572	7.25316	2.62380
7.97511	10.40308	2.62380
10.57568	12.16069	2.62380
9.77796	15.12565	2.62380
12.54209	16.72251	2.62380
7.21729	0.84408	2.62380
9.80054	2.50417	2.62380
10.57160	5.48632	2.62380
13.67369	6.03743	2.62380
13.66694	11.57773	2.62380
15.26840	8.80913	2.62380
14.71136	14.54747	2.62380
17.53265	15.92095	2.62380
12.55360	0.91210	2.62380
14.74234	3.08539	2.62380
18.46588	8.80541	2.62380
20.49431	11.21263	2.62380
20.26145	14.34624	2.62380
22.85078	16.00778	2.62380
17.55783	1.69414	2.62380
20.28509	3.26759	2.62380
20.48945	6.40218	2.62380
23.46354	7.20862	2.62380
23.46220	10.39097	2.62380
26.18930	11.80056	2.62380
25.72718	14.84947	2.62380
28.15159	16.77229	2.62380

Optimized 585 Defect

1.0

20.308350144	0	0.0000000000	
10.154127744	17.58755808	0.0000000000	
0.0000000000	0.0000000000		20.0000000000

Si 0

60 120

Cartesian

2.01895	1.16560	0.99619
4.63612	2.67668	0.99996
5.19714	5.62379	1.00144
8.13339	6.45460	0.99772
8.18866	9.57959	1.02207
10.83700	11.11015	1.02177
10.21308	14.14287	1.00370
12.65861	15.83440	1.00568
7.46892	1.68897	1.00145
9.65656	3.81642	0.99771
13.56791	9.59321	0.99767
15.75124	11.72596	1.00150
15.40081	14.71563	0.99714
17.99680	16.28901	0.99724
12.39052	2.30179	1.02207
15.04021	3.83001	1.02178
15.09194	6.95350	0.99767
18.03061	7.77797	1.00150
18.58223	10.72846	0.99975
21.19731	12.23830	0.99626
20.74325	15.16582	1.00492
23.19581	16.85966	1.00274
17.35467	1.77337	1.00371
20.04236	3.04549	1.00568
20.44455	5.97967	0.99713
23.10510	7.44123	0.99725
23.50558	10.38131	1.00493
26.19879	11.65835	1.00274
25.52018	14.73409	1.01790
28.22102	16.29343	1.01777
2.01895	1.16560	4.25140
4.63612	2.67668	4.24763
5.19714	5.62379	4.24615
8.13339	6.45460	4.24987
8.18866	9.57959	4.22552
10.83700	11.11015	4.22582
10.21308	14.14287	4.24389
12.65861	15.83440	4.24191
7.46892	1.68897	4.24614
9.65656	3.81642	4.24988
13.56791	9.59321	4.24992
15.75124	11.72596	4.24609

15.40081	14.71563	4.25045
17.99680	16.28901	4.25035
12.39052	2.30179	4.22552
15.04021	3.83001	4.22581
15.09194	6.95350	4.24992
18.03061	7.77797	4.24609
18.58223	10.72846	4.24784
21.19731	12.23830	4.25133
20.74325	15.16582	4.24267
23.19581	16.85966	4.24485
17.35467	1.77337	4.24388
20.04236	3.04549	4.24191
20.44455	5.97967	4.25046
23.10510	7.44123	4.25034
23.50558	10.38131	4.24266
26.19879	11.65835	4.24485
25.52018	14.73409	4.22969
28.22102	16.29343	4.22982
3.32980	1.92243	0.42056
4.62501	4.20523	0.45923
5.95437	1.90282	0.45922
6.71788	5.82809	0.47091
8.11818	8.02117	0.45315
9.33957	5.39220	0.52602
9.70414	10.01372	0.66359
10.25783	12.57071	0.46627
12.21929	10.38892	0.45226
11.67722	14.64968	0.52370
14.14147	15.56184	0.43256
12.11706	17.24155	0.42741
8.40625	2.90380	0.47090
11.00565	3.01997	0.45316
14.81565	10.50973	0.47110
13.88786	8.01813	0.52527
15.26271	13.18265	0.45963
17.26588	11.50682	0.46085
16.70466	15.49215	0.43113
19.26679	15.46290	0.43066
7.96014	0.23463	0.45833
13.52421	3.39716	0.66360
15.10677	5.38772	0.45225
16.01551	2.59817	0.46625
16.50954	7.57584	0.47111
18.59813	9.19928	0.46087
19.04788	6.62658	0.45962
19.88752	11.48207	0.41901
21.25445	13.74855	0.42722
22.53382	11.53268	0.42723
21.74430	16.32873	0.51379
24.30742	15.73795	0.46344

12.97521	0.84382	0.46734
18.52568	2.78797	0.52377
20.54774	4.46599	0.43256
20.99022	1.87291	0.42739
21.76892	6.72062	0.43113
23.02463	8.95413	0.43068
4.18326	6.77639	0.45832
25.01322	10.66676	0.51375
25.78319	13.18188	0.46344
7.21835	10.81493	0.46735
26.87069	15.51384	0.62048
9.12300	15.28581	0.46293
17.79947	0.25785	0.46294
3.32980	1.92243	4.82703
4.62501	4.20523	4.78836
5.95437	1.90282	4.78837
6.71788	5.82809	4.77668
8.11818	8.02117	4.79444
9.33957	5.39220	4.72157
9.70414	10.01372	4.58400
10.25783	12.57071	4.78132
12.21929	10.38892	4.79533
11.67722	14.64968	4.72389
14.14147	15.56184	4.81503
12.11706	17.24155	4.82018
8.40625	2.90380	4.77669
11.00565	3.01997	4.79443
14.81565	10.50973	4.77649
13.88786	8.01813	4.72232
15.26271	13.18265	4.78796
17.26588	11.50682	4.78674
16.70466	15.49215	4.81646
19.26679	15.46290	4.81693
7.96014	0.23463	4.78926
13.52421	3.39716	4.58399
15.10677	5.38772	4.79534
16.01551	2.59817	4.78134
16.50954	7.57584	4.77648
18.59813	9.19928	4.78672
19.04788	6.62658	4.78797
19.88752	11.48207	4.82858
21.25445	13.74855	4.82037
22.53382	11.53268	4.82036
21.74430	16.32873	4.73380
24.30742	15.73795	4.78415
12.97521	0.84382	4.78025
18.52568	2.78797	4.72382
20.54774	4.46599	4.81503
20.99022	1.87291	4.82020
21.76892	6.72062	4.81646

23.02463	8.95413	4.81691
4.18326	6.77639	4.78927
25.01322	10.66676	4.73384
25.78319	13.18188	4.78415
7.21835	10.81493	4.78024
26.87069	15.51384	4.62711
9.12300	15.28581	4.78466
17.79947	0.25785	4.78465
2.04494	1.18060	2.62380
4.61745	2.66588	2.62380
5.21382	5.63623	2.62380
8.18236	6.50713	2.62380
7.92116	9.49838	2.62380
11.03963	11.30106	2.62380
10.03349	14.10154	2.62380
12.69042	15.87994	2.62380
7.48802	1.69721	2.62380
9.72655	3.83258	2.62380
13.49675	9.57573	2.62380
15.72825	11.71850	2.62380
15.42878	14.70294	2.62380
17.96810	16.30166	2.62380
12.18643	2.11071	2.62380
15.30686	3.91002	2.62380
15.04124	6.90059	2.62380
18.01266	7.76181	2.62380
18.60012	10.73880	2.62380
21.17164	12.22348	2.62380
20.71376	15.12699	2.62380
23.36490	16.89952	2.62380
17.22906	1.63849	2.62380
20.09777	3.05025	2.62380
20.44750	6.01029	2.62380
23.10173	7.41003	2.62380
23.45726	10.37520	2.62380
26.31780	11.78481	2.62380
25.30657	14.61075	2.62380
28.43825	16.41883	2.62380

Optimized Tetravacancy Defect

1.0

20.566400000	0.0000000000	0.0000000000
10.283200000	17.811000000	0.0000000000
0.0000000000	0.0000000000	10.000000000

Si 0

56 110

Cartesian

2.44959	1.41428	0.99715
4.99473	2.88370	1.00110
5.15513	5.84272	1.00015
8.13201	6.51844	1.00073
8.19407	9.64314	1.00048
10.86413	11.26327	0.99796
9.99762	14.16691	1.01350
12.42630	15.79795	0.99717
7.63751	1.54312	1.00015
9.71118	3.78331	1.00073
14.02619	11.25799	1.00062
14.92710	14.17415	1.00150
17.45491	15.84662	1.00248
12.44824	2.27470	1.00048
15.18632	3.77696	0.99796
16.76279	6.51803	1.00062
16.69653	9.63978	1.00077
19.51744	11.26839	1.00074
20.05397	14.35470	1.00233
22.39171	16.36006	1.03573
17.26773	1.57475	1.01350
19.89461	2.86250	0.99717
19.73875	5.84013	1.00150
22.45109	7.19311	1.00248
22.45854	10.18982	1.00233
25.36405	11.21175	1.03573
24.80677	14.32218	1.44577
27.52168	15.88964	1.41713
2.44959	1.41428	4.25044
4.99473	2.88370	4.24649
5.15513	5.84272	4.24744
8.13201	6.51844	4.24686
8.19407	9.64314	4.24711
10.86413	11.26327	4.24963
9.99762	14.16691	4.23409
12.42630	15.79795	4.25042
7.63751	1.54312	4.24744
9.71118	3.78331	4.24686
14.02619	11.25799	4.24697
14.92710	14.17415	4.24609
17.45491	15.84662	4.24511
12.44824	2.27470	4.24711

15.18632	3.77696	4.24963
16.76279	6.51803	4.24697
16.69653	9.63978	4.24682
19.51744	11.26839	4.24685
20.05397	14.35470	4.24526
22.39171	16.36006	4.21186
17.26773	1.57475	4.23409
19.89461	2.86250	4.25042
19.73875	5.84013	4.24609
22.45109	7.19311	4.24511
22.45854	10.18982	4.24526
25.36405	11.21175	4.21186
24.80677	14.32218	3.80182
27.52168	15.88964	3.83046
3.72276	2.14933	0.38618
4.96932	4.36436	0.41628
6.26430	2.12138	0.41628
6.60653	6.31523	0.45447
8.39728	8.07180	0.52096
9.15633	5.28641	0.49020
9.65372	10.25483	0.51778
10.28273	12.68276	0.42328
12.44533	10.98872	0.49492
11.12798	15.10497	0.36856
13.72508	15.06579	0.43571
12.45595	17.26954	0.38927
8.77240	2.56382	0.45447
11.18904	3.23635	0.52096
14.61392	12.68069	0.45404
15.23750	10.25180	0.51637
16.24369	14.92687	0.42648
18.75853	15.11307	0.46779
7.64289	0.02735	0.42934
13.70780	3.23295	0.51778
15.73915	5.28361	0.49492
16.12496	2.56374	0.42328
16.49709	8.07012	0.51637
18.28878	6.31565	0.45404
18.11042	10.45607	0.49879
19.73223	12.82269	0.49785
20.97092	10.67727	0.49785
21.24501	15.33900	0.41857
23.71000	15.39535	0.80893
12.45422	0.64359	0.48639
18.64530	2.08463	0.36856
19.90992	4.35335	0.43571
21.18380	2.15243	0.38927
21.04890	6.60402	0.42648
22.46759	8.68878	0.46779
3.84507	6.60532	0.42934

23.90652	10.72920	0.41857
25.18782	12.83572	0.80893
6.78445	10.46390	0.48639
26.16357	15.10552	1.12377
8.61115	14.92874	0.66190
17.23424	-0.00682	0.66190
3.72276	2.14933	4.86141
4.96932	4.36436	4.83131
6.26430	2.12138	4.83131
6.60653	6.31523	4.79312
8.39728	8.07180	4.72663
9.15633	5.28641	4.75739
9.65372	10.25483	4.72981
10.28273	12.68276	4.82431
12.44533	10.98872	4.75267
11.12798	15.10497	4.87903
13.72508	15.06579	4.81188
12.45595	17.26954	4.85832
8.77240	2.56382	4.79312
11.18904	3.23635	4.72663
14.61392	12.68069	4.79355
15.23750	10.25180	4.73122
16.24369	14.92687	4.82111
18.75853	15.11307	4.77980
7.64289	0.02735	4.81825
13.70780	3.23295	4.72981
15.73915	5.28361	4.75267
16.12496	2.56374	4.82431
16.49709	8.07012	4.73122
18.28878	6.31565	4.79355
18.11042	10.45607	4.74880
19.73223	12.82269	4.74974
20.97092	10.67727	4.74974
21.24501	15.33900	4.82902
23.71000	15.39535	4.43866
12.45422	0.64359	4.76120
18.64530	2.08463	4.87903
19.90992	4.35335	4.81188
21.18380	2.15243	4.85832
21.04890	6.60402	4.82111
22.46759	8.68878	4.77980
3.84507	6.60532	4.81825
23.90652	10.72920	4.82902
25.18782	12.83572	4.43866
6.78445	10.46390	4.76120
26.16357	15.10552	4.12382
8.61115	14.92874	4.58569
17.23424	-0.00682	4.58569
2.44977	1.41437	2.62380
4.99941	2.88641	2.62380

5.16471	5.90926	2.62380
8.17587	6.46323	2.62380
8.11347	9.69582	2.62380
10.92322	11.25409	2.62380
10.12543	14.06252	2.62380
12.40430	15.79574	2.62380
7.69993	1.51814	2.62380
9.68528	3.84889	2.62380
13.96193	11.24261	2.62380
14.98939	14.12841	2.62380
17.35217	15.89947	2.62380
12.45355	2.17856	2.62380
15.20793	3.83272	2.62380
16.71733	6.47008	2.62380
16.77770	9.68663	2.62380
19.44021	11.22379	2.62380
20.21586	14.29644	2.62380
22.10725	16.54315	2.62380
17.24125	1.73763	2.62380
19.88170	2.84455	2.62380
19.73028	5.91695	2.62380
22.44549	7.07771	2.62380
22.48902	10.35915	2.62380
25.38038	10.87386	2.62380