

# Theoretical and Experimental Exploration of the Anisotropy of Styrene Diffusion on Hydrogen Terminated Si(100)-2×1

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## **Supplementary Information:**

**Table S1.** Cartesian coordinates of the two lowest energy optimized structures of styrene on H-Si(100)-2x1, in Å.

- |    |                        |      |
|----|------------------------|------|
| a) | Structure for Fig 1(a) | p S2 |
| b) | Structure for Fig 1(b) | p S5 |

**Figure S1.** Sample input file demonstrating the use of dispersion-correcting potential with the Gaussian-03 program package. The input represents the structure shown in Figure 2 of the manuscript.

p S8

## **Also Available Online:**

MC movie of a Two Dose Styrene Simulation

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**Table S1.** Cartesian coordinates of the two lowest energy optimized structures of styrene on H-Si(100)-2x1, in Å. Data are *atom type, x-coordinate, y-coordinate, z-coordinate*.  
(a) Structure for Fig 1(a).

Si	-7.88103	5.755571	0.161065
Si	-7.79818	-1.94442	-0.39092
Si	-7.84195	2.128167	-0.0991
Si	-7.75929	-5.57186	-0.65058
Si	-7.84761	0.180546	-1.48666
Si	-5.91988	5.07748	1.293446
Si	-2.06086	5.124602	1.215366
Si	1.797722	5.171667	1.137317
Si	5.656743	5.218684	1.059281
Si	-5.83702	-2.62251	0.741465
Si	-1.978	-2.57539	0.663385
Si	1.880376	-2.52832	0.58534
Si	5.739396	-2.48131	0.507305
Si	-5.89401	2.679682	1.121383
Si	-2.03499	2.726703	1.043295
Si	1.823389	2.773765	0.96525
Si	5.682408	2.820884	0.887222
Si	-5.81134	-5.02034	0.569908
Si	-1.95232	-4.97332	0.49182
Si	1.906255	-4.92626	0.413771
Si	5.765274	-4.87914	0.335743
Si	-4.02201	5.802693	0.082984
Si	-0.16382	5.849804	0.004921
Si	3.694374	5.896812	-0.0731
Si	7.553395	5.943829	-0.15113
Si	-3.93916	-1.8973	-0.469
Si	-0.08107	-1.85019	-0.54706
Si	3.777028	-1.80318	-0.62508
Si	7.636048	-1.75616	-0.70311
Si	-3.98293	2.175188	-0.17719
Si	-0.12484	2.222198	-0.25526
Si	3.733257	2.269305	-0.33327
Si	7.592276	2.316423	-0.4113
Si	-3.90027	-5.52484	-0.72867
Si	-0.04207	-5.47783	-0.80674
Si	3.816122	-5.43072	-0.88475
Si	7.675142	-5.3836	-0.96278
Si	-3.98859	0.227618	-1.56474
Si	-0.12915	0.274695	-1.64283
Si	3.730289	0.321768	-1.72087
Si	7.589309	0.368835	-1.79891
Si	-5.9491	0.304122	-2.92652
Si	-2.09008	0.351193	-3.0046
Si	1.772674	0.398309	-3.08274
Si	5.631694	0.445377	-3.16077
H	-5.90774	5.504001	2.734118

H	-2.04872	5.551123	2.656037
H	1.833449	5.598475	2.577511
H	5.692469	5.645493	2.499476
H	-5.82488	-2.19599	2.182137
H	-1.96586	-2.14887	2.104057
H	1.916102	-2.10152	2.025535
H	5.775122	-2.0545	1.947499
H	-5.87055	2.052497	2.486553
H	-2.01153	2.099518	2.408466
H	1.87044	2.146868	2.329944
H	5.72946	2.193986	2.251915
H	-5.78788	-5.64753	1.935078
H	-1.92886	-5.60051	1.856991
H	1.953306	-5.55316	1.778464
H	5.812326	-5.50604	1.700436
H	7.524652	7.250111	-0.8252
H	3.665634	7.202989	-0.74712
H	-0.19338	7.155867	-0.66904
H	-4.0524	7.108849	-0.59101
H	-7.91142	7.061832	-0.51297
H	7.673306	-6.58076	-1.81623
H	3.814287	-6.62778	-1.73814
H	-0.04473	-6.6748	-1.66005
H	-3.90375	-6.72192	-1.58202
H	-7.76277	-6.76904	-1.50399
H	-9.0607	5.304797	0.913458
H	-9.03011	2.439069	0.70374
H	-8.97819	-2.39193	0.357585
H	-8.94716	-5.25828	0.156583
H	8.855917	-2.1744	-0.00315
H	8.886687	-5.04075	-0.20415
H	8.803993	2.656598	0.343003
H	8.773155	5.522322	0.552725
H	5.622149	-0.65209	-4.14141
H	1.76313	-0.69921	-4.06333
H	-2.09344	-0.74625	-3.98532
H	-5.95246	-0.79327	-3.90728
H	-5.97743	1.529797	-3.74083
H	-2.11841	1.576915	-3.81886
H	1.738161	1.623955	-3.89687
H	5.59718	1.670976	-3.97495
H	8.758148	0.444968	-2.6861
H	-9.05287	0.227721	-2.32583
H	7.629638	-2.81987	-1.7177
H	3.770618	-2.86691	-1.63963
H	3.785334	-4.23471	-1.73886
H	-0.08861	-2.91396	-1.56157
H	-0.07394	-4.28183	-1.66083
H	-3.94784	-2.96106	-1.48351
H	-3.93321	-4.32885	-1.58273

H	-7.80686	-3.00815	-1.40546
H	-7.79223	-4.37587	-1.50465
H	7.644354	-4.18759	-1.81689
H	7.546881	4.881409	-1.16707
H	7.561567	3.513519	-1.26389
H	3.68786	4.834392	-1.08903
H	3.702548	3.466424	-1.18583
H	-0.17141	4.787371	-1.01099
H	-0.15668	3.419327	-1.10777
H	-4.03068	4.740246	-0.93291
H	-4.01591	3.37228	-1.02971
H	-7.8897	4.693124	-0.85483
H	-7.87493	3.325235	-0.95165
C	2.502915	-2.81035	4.658658
C	3.247277	-1.62001	4.536359
C	1.085204	-2.80262	4.577227
H	3.021491	-3.75799	4.806054
C	2.586245	-0.39206	4.33301
H	4.33446	-1.65353	4.591954
C	0.433021	-1.55302	4.387342
C	1.174901	-0.36527	4.264226
H	3.157087	0.529666	4.230278
H	-0.65304	-1.50978	4.3283
H	0.656073	0.580428	4.112327
C	0.355467	-4.09599	4.670746
H	0.995714	-4.96565	4.837292
C	-0.97606	-4.29851	4.562393
H	-1.68509	-3.49012	4.390682
H	-1.39195	-5.30026	4.644881

(a) Structure for Fig 1(b).

Si	7.707109	-5.69695	-0.52015
Si	7.842437	2.014043	-0.16849
Si	7.770811	-2.06434	-0.35462
Si	7.906331	5.646621	-0.00245
Si	7.831424	0.03117	-1.50514
Si	5.76616	-5.10096	0.690532
Si	1.907343	-5.03007	0.620942
Si	-1.95103	-4.95913	0.551388
Si	-5.80985	-4.88813	0.481854
Si	5.901489	2.610029	1.042195
Si	2.042672	2.680925	0.972604
Si	-1.8155	2.751859	0.903054
Si	-5.67432	2.822853	0.83352
Si	5.808236	-2.69972	0.799867
Si	1.94942	-2.62872	0.730281
Si	-1.90875	-2.55779	0.660732
Si	-5.76757	-2.48689	0.591193
Si	5.943757	5.011249	1.152036
Si	2.084941	5.082246	1.08245
Si	-1.77344	5.153184	1.012897
Si	-5.63225	5.224077	0.943357
Si	3.848291	-5.62605	-0.58974
Si	-0.0097	-5.55517	-0.65931
Si	-3.86769	-5.48419	-0.72883
Si	-7.72651	-5.4132	-0.79837
Si	3.98362	2.084939	-0.23808
Si	0.12573	2.155818	-0.30765
Si	-3.73216	2.226796	-0.37717
Si	-7.59098	2.297791	-0.4467
Si	3.911995	-1.99335	-0.4242
Si	0.054106	-1.92237	-0.49377
Si	-3.80379	-1.85149	-0.56329
Si	-7.6626	-1.7806	-0.63283
Si	4.047516	5.717618	-0.07203
Si	0.189526	5.7886	-0.1416
Si	-3.66847	5.859478	-0.21113
Si	-7.52728	5.930372	-0.28067
Si	3.972607	0.102117	-1.57473
Si	0.113373	0.17307	-1.64433
Si	-3.74586	0.244022	-1.71387
Si	-7.60468	0.314967	-1.78341
Si	5.929927	0.130184	-2.94295
Si	2.07111	0.20113	-3.01254
Si	-1.79144	0.272144	-3.08217
Si	-5.65026	0.343089	-3.15171
H	5.742193	-5.69243	2.071542
H	1.883376	-5.62154	2.001953
H	-1.99859	-5.55017	1.931974

H	-5.85741	-5.47917	1.86244
H	5.877521	2.018557	2.423205
H	2.018703	2.089453	2.353615
H	-1.86306	2.160821	2.283639
H	-5.72188	2.231816	2.214106
H	5.8028	-2.23598	2.229035
H	1.943985	-2.16498	2.159449
H	-1.93778	-2.09362	2.089474
H	-5.7966	-2.02272	2.019936
H	5.938321	5.474986	2.581203
H	2.079506	5.545982	2.511618
H	-1.80246	5.617353	2.441639
H	-5.66128	5.688247	2.372101
H	-7.73492	-6.63203	-1.62053
H	-3.8761	-6.70292	-1.55094
H	-0.01729	-6.77382	-1.48135
H	3.841529	-6.84482	-1.41181
H	7.700346	-6.91581	-1.34228
H	-7.49167	7.218547	-0.98841
H	-3.63285	7.147551	-0.91882
H	0.225962	7.076554	-0.84924
H	4.084779	7.005659	-0.7797
H	7.943597	6.934767	-0.71016
H	8.899209	-5.37057	0.275636
H	8.949825	-2.50025	0.402259
H	9.03479	2.337635	0.623052
H	9.084987	5.20756	0.758404
H	-8.79838	2.665501	0.301577
H	-8.74793	5.535423	0.436934
H	-8.88334	-2.17238	0.080785
H	-8.93371	-5.0427	-0.04583
H	-5.60979	1.546946	-3.99744
H	-1.75097	1.476049	-3.92785
H	2.105397	1.40515	-3.85834
H	5.964214	1.334154	-3.7888
H	5.923357	-0.99222	-3.89497
H	2.064539	-0.92133	-3.96451
H	-1.79183	-0.85043	-4.03403
H	-5.65064	-0.77943	-4.10361
H	-8.77536	0.375958	-2.66934
H	9.034717	0.048517	-2.34828
H	-7.5546	3.472186	-1.33009
H	-3.69578	3.401216	-1.26052
H	-3.67174	4.771101	-1.19922
H	0.163245	3.330241	-1.19095
H	0.187327	4.700202	-1.12968
H	4.022273	3.259317	-1.12139
H	4.046393	4.629201	-1.06009
H	7.881091	3.188397	-1.05183
H	7.905209	4.558204	-0.9905

H	-7.53056	4.841994	-1.26876
H	-7.69006	-4.23992	-1.68324
H	-7.66599	-2.87022	-1.61954
H	-3.83125	-4.31092	-1.61371
H	-3.80717	-2.94114	-1.54997
H	0.027822	-4.38192	-1.54417
H	0.051858	-3.01207	-1.4804
H	3.886889	-4.45282	-1.47457
H	3.910886	-3.08304	-1.41084
H	7.745706	-4.52371	-1.40498
H	7.769701	-3.15401	-1.34129
C	-2.0989	-0.50316	4.374572
C	-3.18968	-1.3803	4.530856
C	-0.76148	-0.98401	4.392596
H	-2.27884	0.563031	4.236486
C	-2.96554	-2.76146	4.704611
H	-4.2061	-0.98953	4.511311
C	-0.55329	-2.38045	4.561741
C	-1.642	-3.25596	4.718929
H	-3.80612	-3.444	4.819598
H	0.458338	-2.783	4.554259
H	-1.46174	-4.32318	4.840903
C	0.355242	-0.01527	4.221976
H	0.048881	0.984665	3.904786
C	1.670148	-0.24443	4.430854
H	2.053051	-1.20541	4.771739
H	2.403429	0.543503	4.272507

**Figure S1.** Sample input file demonstrating the use of dispersion-correcting potential with the Gaussian-03 program package. The input represents the structure shown in Figure 2 of the manuscript.

```
%nproc=2
%mem=7GB
#b971 gen pseudo=read
```

Input demonstrating the use of dispersion-correcting potentials.

```
0 1
14 1.818336956 7.719366373 -1.21885614
14 -5.901854913 7.719263336 -1.218300432
14 -1.818594994 7.719264514 -1.218726905
14 -9.538786509 7.719364204 -1.217669246
14 -3.860354484 7.720609371 -2.46362761
14 1.202050996 5.789924383 0.000025667
14 1.202101748 1.929827403 -0.000000028
14 1.202102241 -1.929827403 0.000000028
14 1.202052532 -5.789923199 0.000027467
14 -6.518141864 5.789821344 0.000580366
14 -6.518090094 1.929726366 0.000555649
14 -6.518088894 -1.929727394 0.000556608
14 -6.518139594 -5.789823191 0.000583038
14 -1.202052349 5.789822988 0.00002559
14 -1.202102606 1.929726388 0.000000028
14 -1.202101384 -1.929726388 -0.000000028
14 -1.202050075 -5.789822578 0.000026278
14 -8.922243864 5.789922677 0.001083249
14 -8.92229413 1.929826093 0.001058687
14 -8.922293637 -1.929828714 0.001058743
14 -8.922242351 -5.789925889 0.001086064
14 1.818388722 3.85927038 -1.218881841
14 1.818439638 -0.00000044 -1.218908286
14 1.818390098 -3.85926906 -1.218880613
14 1.818339384 -7.719365857 -1.218854167
14 -5.901803143 3.859168358 -1.218325149
14 -5.901751857 -0.000001454 -1.21835215
14 -5.901802041 -3.859170052 -1.218325026
14 -5.901851764 -7.719266847 -1.218297572
14 -1.818644237 3.8591689 -1.218752474
14 -1.818693969 -0.000000516 -1.218778341
14 -1.818643144 -3.859169495 -1.218751351
14 -1.818591822 -7.719264685 -1.21872506
14 -9.538836775 3.859267619 -1.217693808
14 -9.538885854 -0.000001834 -1.217720126
```



14	-9.538835376	-3.859270836	-1.217693594
14	-9.538784076	-7.719367011	-1.217666289
14	-3.860353726	3.860513067	-2.463653742
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14	-3.860352961	-3.860514882	-2.46365211
14	-3.860352668	-7.720611368	-2.463625235
1	1.730431645	5.80172146	1.40653706
1	1.730483424	1.941626466	1.406511343
1	1.730483231	-1.941624276	1.40651258
1	1.730433517	-5.801721086	1.406539034
1	-5.989760211	5.801619423	1.407092752
1	-5.989708445	1.94152343	1.407067051
1	-5.989707895	-1.941524282	1.40706816
1	-5.989758609	-5.801621079	1.407094606
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1	-1.730188569	1.94152446	1.406622315
1	-1.730188032	-1.941524251	1.40662344
1	-1.730136723	-5.801620442	1.406649746
1	-9.450330849	5.801719779	1.407706543
1	-9.450380093	1.941624165	1.407680975
1	-9.450380277	-1.941626593	1.407681212
1	-9.450328963	-5.801721768	1.407708502
1	-10.79386542	-7.720192897	-1.983393021
1	-10.79381516	-3.860096298	-1.983367459
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1	-10.79381625	3.860093493	-1.983368157
1	-10.79386757	7.720188669	-1.983395447
1	1.435237069	8.9194135	-0.461213426
1	-1.438313371	8.9195392	-0.465285002
1	-6.281977344	8.919537771	-0.464779483
1	-9.155527565	8.919411351	-0.460106806
1	-6.281975763	-8.919540287	-0.464775871
1	-9.155524572	-8.919414686	-0.460104073
1	-1.438310786	-8.919539902	-0.465283366
1	1.435239062	-8.919412524	-0.461210701
1	-3.860442589	-8.907992998	-3.329198168
1	-3.860445072	8.907990206	-3.329202335
1	-7.035314014	-7.720403125	-2.154334104
1	-7.035289602	-3.860308498	-2.154329735
1	-8.406756176	-3.860347588	-2.155400998
1	-7.035266319	-0.0000008	-2.154324665
1	-8.4068071	-0.000001363	-2.15542816
1	-7.035290962	3.860305377	-2.154330981
1	-8.40675748	3.8603443	-2.155402448
1	-7.035316467	7.720400541	-2.154336047
1	-8.406707237	7.7204399	-2.155376871

1	-8.406704867	-7.720443778	-2.155374693
1	0.68606463	-7.720442298	-2.156325721
1	-0.685324831	-7.720402665	-2.154997169
1	0.686115344	-3.860345501	-2.156352167
1	-0.685351399	-3.860306349	-2.154993261
1	0.686164429	0.000000358	-2.15637947
1	-0.685376142	-0.000001017	-2.154989564
1	0.686114017	3.860345403	-2.156352601
1	-0.685352773	3.860306527	-2.154994492
1	0.686062273	7.72044238	-2.156327915
1	-0.68532827	7.720402015	-2.154999137
14	5.90159671	7.71926668	-1.219534096
14	3.859837219	7.720611537	-2.464434801
14	3.859837978	3.860515233	-2.464460933
14	3.859838091	0.000001871	-2.464485633
14	3.859838729	-3.860513716	-2.464459286
14	3.859839036	-7.720609202	-2.464432426
14	6.518139341	5.789824154	-0.000781586
14	6.518089098	1.929728554	-0.000807163
14	6.518090306	-1.929725222	-0.000807204
14	6.518141615	-5.789821412	-0.000780898
14	5.901547453	3.859170066	-1.219559649
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6	-5.307551838	0.185000304	3.899938826

H C Si 0  
6-31+G(d,p)  
\*\*\*\*

C 0  
C 3 0  
F and up  
2  
2 0.08 -0.0015  
2 0.12 0.0035  
S - F  
1  
2 1.0 0.0  
P - F  
1  
2 1.0 0.0  
D - F  
1  
2 1.0 0.0  
Si 0  
Si 3 0  
F and up  
2  
2 0.04 -0.00051  
2 0.08 0.00165  
S - F  
1  
2 1.0 0.0  
P - F  
1  
2 1.0 0.0  
D - F  
1  
2 1.0 0.0