Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information

for

Regioselectivity Control of Graphene Functionalization by Ripples

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S1. Profiles of the rippled graphene sheets

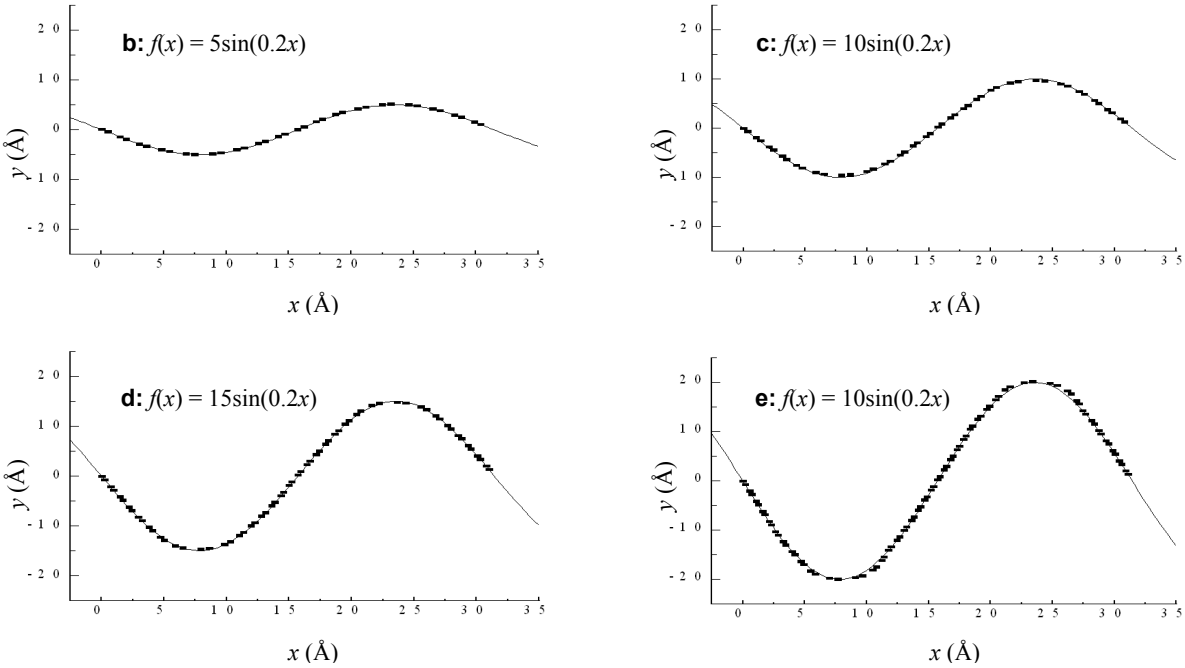

Figure S1. The comparative illustrations of the calculated profiles of the rippled graphene sheets and the ideal sine functions. Dark squares: The side-view profiles of rippled graphene sheets (**b**−**e**) optimized at GGA-PBE/DZP level. Smooth curves: curves of the respective sine functions of the figures.

S2. Optimized Cartesian Coordinates (GGA-PBE/DZP)

a, y = 0

C	0.66996	0.52562	0.49150
C	1.38041	0.48778	1.73537
C	2.80345	0.48601	1.73850

C	3.51441	0.52046	0.49377
C	4.95454	0.56933	0.49302
C	5.67671	0.56823	1.73772
C	7.09791	0.51512	1.73504
C	7.81170	0.48537	0.48991
C	9.24217	0.47654	0.48941
C	9.96577	0.47848	1.73252
C	11.39868	0.47952	1.73157
C	12.11395	0.47853	0.48839
C	13.53653	0.49419	0.48992
C	14.25467	0.53544	1.73400
C	15.69399	0.57093	1.73600
C	16.41072	0.58088	0.49192
C	17.83397	0.58285	0.49072
C	18.55017	0.58292	1.73493
C	19.98109	0.58229	1.73316
C	20.70506	0.58130	0.48886
C	22.13535	0.58525	0.48821
C	22.84796	0.58846	1.73148
C	24.27479	0.58564	1.73072
C	24.99602	0.58329	0.48750
C	26.43758	0.58543	0.48916
C	27.14817	0.59013	1.73347
C	28.57239	0.58845	1.73665
C	29.28413	0.57446	0.49250

LatticeVectors

30.057602	0.000000	0.000000
0.000000	100.000000	0.000000
0.000000	0.000000	2.487311

b, y = 5sin(0.2x)

C	0.05579	-0.03604	1.19371
C	0.55570	0.46830	-0.05169
C	1.52613	1.51069	-0.05176
C	2.02186	2.01763	1.19362
C	3.08038	2.96606	1.19367
C	3.63626	3.38908	-0.05171
C	4.85796	4.12288	-0.05170
C	5.48555	4.44076	1.19369
C	6.81763	4.94220	1.19368
C	7.50831	5.05387	-0.05174
C	8.93191	4.95073	-0.05191
C	9.59992	4.74256	1.19346
C	10.87612	4.11277	1.19331
C	11.46464	3.72099	-0.05213
C	12.60893	2.87769	-0.05217
C	13.14837	2.43816	1.19324
C	14.20720	1.49233	1.19327

C	14.72014	1.00458	-0.05212
C	15.76376	0.03604	-0.05196
C	16.26366	-0.46832	1.19351
C	17.23405	-1.51076	1.19369
C	17.72975	-2.01774	-0.05169
C	18.78840	-2.96608	-0.05136
C	19.34431	-3.38909	1.19414
C	20.56593	-4.12303	1.19428
C	21.19361	-4.44082	-0.05112
C	22.52578	-4.94223	-0.05117
C	23.21643	-5.05387	1.19420
C	24.64001	-4.95072	1.19400
C	25.30800	-4.74257	-0.05142
C	26.58417	-4.11278	-0.05150
C	27.17263	-3.72098	1.19386
C	28.31688	-2.87767	1.19379
C	28.85633	-2.43816	-0.05162
C	29.91516	-1.49235	-0.05166
C	30.42811	-1.00460	1.19373

LatticeVectors
31.4159 0.0000 0.0000
0.0000 100.0000 0.0000
0.0000 0.0000 2.490814

c, y = 10sin(0.2x)

C	0.05166	0.13099	1.24285
C	0.37529	0.77307	0.00002
C	1.08232	2.02842	0.00001
C	1.42304	2.65660	1.24283
C	2.13562	3.90661	1.24283
C	2.47208	4.53707	0.00000
C	3.18197	5.79072	0.00000
C	3.52596	6.42191	1.24282
C	4.32834	7.62955	1.24282
C	4.78354	8.18404	0.00000
C	5.90306	9.10364	0.00001
C	6.55141	9.41786	1.24283
C	7.97970	9.63291	1.24283
C	8.68821	9.52339	0.00001
C	9.98696	8.89802	0.00000
C	10.52813	8.42576	1.24282
C	11.47471	7.34752	1.24282
C	11.89800	6.76976	-0.00001
C	12.70053	5.57379	-0.00003
C	13.04999	4.94958	1.24278
C	13.76425	3.70047	1.24277
C	14.10316	3.07101	-0.00006
C	14.80881	1.81498	-0.00009

C	15.13247	1.17295	1.24273
C	15.75962	-0.13137	1.24272
C	16.08328	-0.77330	-0.00011
C	16.79033	-2.02851	-0.00008
C	17.13103	-2.65664	1.24275
C	17.84357	-3.90660	1.24277
C	18.18000	-4.53702	-0.00005
C	18.88984	-5.79056	-0.00004
C	19.23373	-6.42166	1.24278
C	20.03577	-7.62914	1.24279
C	20.49056	-8.18374	-0.00003
C	21.60925	-9.10349	-0.00002
C	22.25683	-9.41773	1.24281
C	23.68314	-9.63311	1.24281
C	24.39041	-9.52461	-0.00001
C	25.69301	-8.90707	0.00000
C	26.24175	-8.45009	1.24283
C	27.18243	-7.35915	1.24282
C	27.60723	-6.78300	0.00000
C	28.40485	-5.57794	0.00001
C	28.75575	-4.95203	1.24284
C	29.47110	-3.70176	1.24284
C	29.81035	-3.07187	0.00003
C	30.51652	-1.81557	0.00003
C	30.84031	-1.17355	1.24285

LatticeVectors

31.41590	0.00000	0.00000
0.00000	100.00000	0.00000
0.00000	0.00000	2.48564

d, y = 15sin(0.2x)

C	0.05423	0.16122	1.18837
C	0.27182	0.85961	-0.05182
C	0.76875	2.22103	-0.05178
C	1.00671	2.90039	1.18842
C	1.50865	4.25935	1.18845
C	1.73949	4.94945	-0.05176
C	2.23870	6.31167	-0.05179
C	2.46916	7.00600	1.18840
C	2.99061	8.35705	1.18833
C	3.28287	9.01858	-0.05186
C	3.83021	10.35493	-0.05181
C	4.12986	11.01204	1.18840
C	4.73317	12.32669	1.18844
C	5.06483	12.96651	-0.05174
C	5.93659	14.10812	-0.05172
C	6.54317	14.50688	1.18846
C	7.96169	14.74969	1.18844

C	8.66532	14.61020	-0.05178
C	9.87021	13.81313	-0.05182
C	10.32864	13.26683	1.18836
C	11.06067	12.02979	1.18831
C	11.37801	11.38298	-0.05189
C	11.99123	10.07061	-0.05186
C	12.29549	9.41539	1.18835
C	12.84541	8.07847	1.18842
C	13.13667	7.41430	-0.05178
C	13.65878	6.06131	-0.05171
C	13.89239	5.36766	1.18848
C	14.38772	4.00046	1.18843
C	14.60498	3.29840	-0.05178
C	15.03056	1.91284	-0.05178
C	15.24814	1.21127	1.18842
C	15.74456	-0.15441	1.18849
C	15.97805	-0.84499	-0.05169
C	16.48010	-2.20562	-0.05162
C	16.71644	-2.88618	1.18857
C	17.21726	-4.24733	1.18862
C	17.44653	-4.94245	-0.05159
C	17.94574	-6.30662	-0.05162
C	18.17717	-7.00057	1.18856
C	18.69878	-8.35274	1.18850
C	18.99077	-9.01611	-0.05171
C	19.53747	-10.35354	-0.05177
C	19.83603	-11.01135	1.18845
C	20.43399	-12.32819	1.18847
C	20.76964	-12.96692	-0.05171
C	21.64351	-14.10745	-0.05169
C	22.25009	-14.50645	1.18851
C	23.66815	-14.74997	1.18846
C	24.37196	-14.61037	-0.05174
C	25.57672	-13.81257	-0.05188
C	26.03601	-13.26635	1.18833
C	26.76855	-12.02879	1.18833
C	27.08594	-11.38100	-0.05185
C	27.69990	-10.06774	-0.05182
C	28.00476	-9.41140	1.18839
C	28.55408	-8.07183	1.18842
C	28.84287	-7.40155	-0.05178
C	29.36353	-6.04631	-0.05181
C	29.59816	-5.35709	1.18838
C	30.09902	-3.99155	1.18834
C	30.32989	-3.29269	-0.05186
C	30.82637	-1.92410	-0.05187
C	31.04482	-1.22365	1.18833

LatticeVectors
31.4159 0.0000 0.0000
0.0000 100.0000 0.0000

0.0000 0.0000 2.480394

e, y = 20sin(0.2x)

C	0.06315	0.12132	1.19408
C	0.25138	0.79239	-0.05186
C	0.58845	2.17097	-0.05167
C	0.77359	2.85104	1.19449
C	1.11139	4.22842	1.19515
C	1.29663	4.90819	-0.05032
C	1.63402	6.28728	-0.04797
C	1.82241	6.95864	1.20003
C	2.15677	8.34069	1.21082
C	2.34227	9.01613	-0.02778
C	2.68067	10.39483	0.02823
C	2.87421	11.07510	1.28175
C	3.29499	12.43267	1.29207
C	3.51923	13.09201	0.04804
C	4.02068	14.42443	0.05053
C	4.25277	15.08481	1.29706
C	4.74078	16.42408	1.29768
C	4.95789	17.09995	0.05182
C	5.50335	18.41120	0.05196
C	5.90407	19.00170	1.29797
C	7.03835	19.86603	1.29779
C	7.72267	20.05070	0.05165
C	9.12543	19.75003	0.05097
C	9.69777	19.33621	1.29652
C	10.54125	18.19180	1.29403
C	10.83943	17.55633	0.04602
C	11.26964	16.20464	0.03511
C	11.45554	15.53058	1.27382
C	11.79385	14.15142	1.21842
C	12.00449	13.48576	-0.03493
C	12.49548	12.15233	-0.04579
C	12.70977	11.49246	1.19832
C	13.05918	10.11924	1.19614
C	13.25014	9.44248	-0.04993
C	13.66371	8.08537	-0.04809
C	13.86520	7.42066	1.19969
C	14.20567	6.04307	1.20936
C	14.38938	5.36694	-0.02976
C	14.72550	3.99044	0.02404
C	14.90985	3.30979	1.27725
C	15.24758	1.93243	1.28682
C	15.43521	1.25932	0.04087
C	15.77117	-0.12139	0.03196
C	15.95929	-0.79278	1.27116
C	16.29641	-2.17104	1.21648

C	16.48152	-2.85149	-0.03671
C	16.81933	-4.22898	-0.04664
C	17.00441	-4.90896	1.19750
C	17.34187	-6.28794	1.19530
C	17.53031	-6.95939	-0.05117
C	17.86473	-8.34130	-0.05158
C	18.05039	-9.01619	1.19432
C	18.38869	-10.39521	1.19439
C	18.58225	-11.07514	-0.05160
C	19.00297	-12.43259	-0.05145
C	19.22723	-13.09197	1.19453
C	19.72869	-14.42427	1.19419
C	19.96071	-15.08465	-0.05188
C	20.44849	-16.42400	-0.05190
C	20.66576	-17.09980	1.19410
C	21.21124	-18.41103	1.19397
C	21.61188	-19.00159	-0.05213
C	22.74590	-19.86595	-0.05194
C	23.43022	-20.05076	1.19410
C	24.83292	-19.75017	1.19419
C	25.40547	-19.33640	-0.05187
C	26.24902	-18.19205	-0.05171
C	26.54734	-17.55658	1.19430
C	26.97762	-16.20501	1.19425
C	27.16357	-15.53150	-0.05181
C	27.50181	-14.15190	-0.05182
C	27.71220	-13.48619	1.19424
C	28.20330	-12.15270	1.19415
C	28.41780	-11.49273	-0.05187
C	28.76735	-10.11949	-0.05195
C	28.95822	-9.44253	1.19406
C	29.37168	-8.08524	1.19409
C	29.57317	-7.42032	-0.05189
C	29.91354	-6.04266	-0.05181
C	30.09736	-5.36688	1.19416
C	30.43336	-3.99008	1.19418
C	30.61780	-3.30952	-0.05186
C	30.95544	-1.93235	-0.05188
C	31.14319	-1.25913	1.19412

LatticeVectors

31.415900	0.000000	0.000000
0.000000	100.000000	0.000000
0.000000	0.000000	2.492030

f, y = 10sin(0.2x)

C	0.58564	1.17425	-0.04737
C	0.58563	1.17427	1.38891
C	0.05178	0.04937	2.10233

C	0.05182	0.04942	3.54361
C	1.74095	3.38122	-0.04996
C	1.74097	3.38126	1.39140
C	1.19079	2.26301	2.10559
C	1.19078	2.26297	3.54028
C	2.97587	5.55892	-0.04712
C	2.97583	5.55884	1.38852
C	2.35600	4.46365	2.10430
C	2.35600	4.46368	3.54162
C	4.33604	7.64658	-0.04754
C	4.33602	7.64655	1.38836
C	3.61813	6.62283	2.10197
C	3.61812	6.62281	3.54344
C	6.14057	9.33497	-0.04922
C	6.14057	9.33496	1.38922
C	5.16526	8.58087	2.10582
C	5.16522	8.58086	3.53903
C	8.54226	9.82544	-0.04375
C	8.54223	9.82547	1.38287
C	7.28448	9.83080	2.10758
C	7.28443	9.83077	3.53639
C	10.63470	8.49353	-0.05029
C	10.63469	8.49354	1.38870
C	9.68663	9.31029	2.10120
C	9.68660	9.31029	3.54190
C	12.18933	6.52537	-0.05127
C	12.18929	6.52544	1.38949
C	11.46600	7.55062	2.10358
C	11.46601	7.55060	3.53916
C	13.46076	4.37961	-0.04909
C	13.46078	4.37971	1.38662
C	12.83461	5.46464	2.10290
C	12.83456	5.46468	3.53943
C	14.62133	2.16927	-0.04985
C	14.62131	2.16929	1.38675
C	14.07068	3.28552	2.09982
C	14.07067	3.28551	3.54178
C	15.75974	-0.04981	-0.05236
C	15.75975	-0.04983	1.38895
C	15.22565	1.07777	2.10316
C	15.22562	1.07782	3.53799
C	16.89955	-2.26275	-0.04882
C	16.89955	-2.26274	1.38578
C	16.29391	-1.17431	2.10252
C	16.29391	-1.17434	3.53873
C	18.06412	-4.46350	-0.04990
C	18.06415	-4.46363	1.38737
C	17.44932	-3.38105	2.10007
C	17.44934	-3.38105	3.54136
C	19.32605	-6.62293	-0.05177

C	19.32610	-6.62297	1.38974
C	18.68374	-5.55900	2.10335
C	18.68373	-5.55893	3.53898
C	20.87325	-8.58092	-0.04724
C	20.87322	-8.58092	1.38595
C	20.04407	-7.64664	2.10345
C	20.04405	-7.64663	3.53936
C	22.99239	-9.83066	-0.04489
C	22.99234	-9.83063	1.38386
C	21.84857	-9.33485	2.10243
C	21.84861	-9.33487	3.54083
C	25.39448	-9.31040	-0.05064
C	25.39447	-9.31038	1.39007
C	24.25007	-9.82545	2.10847
C	24.25009	-9.82546	3.53515
C	27.17384	-7.55086	-0.04747
C	27.17389	-7.55080	1.38800
C	26.34254	-8.49370	2.10262
C	26.34259	-8.49366	3.54162
C	28.54245	-5.46539	-0.04753
C	28.54246	-5.46536	1.38886
C	27.89720	-6.52587	2.10239
C	27.89721	-6.52585	3.54306
C	29.77824	-3.28630	-0.05021
C	29.77824	-3.28630	1.39177
C	29.16898	-4.38140	2.10514
C	29.16899	-4.38140	3.54082
C	30.93350	-1.07835	-0.04664
C	30.93349	-1.07837	1.38831
C	30.32933	-2.17044	2.10470
C	30.32936	-2.17037	3.54139

LatticeVectors

31.415900	0.000000	0.000000
0.000000	100.000000	0.000000
0.000000	0.000000	4.304417

hydride of **b**

C	0.05626	-0.03532	1.19663
C	2.03067	2.02197	1.19663
C	3.09028	2.96489	1.19663
C	5.52116	4.44142	1.19663
C	6.76491	5.06357	1.19663
C	9.56671	4.73297	1.19663
C	10.85439	4.09696	1.19664
C	13.14725	2.44071	1.19664
C	14.20677	1.49393	1.19663
C	16.26744	-0.47049	1.19663
C	17.23649	-1.51235	1.19663

C	19.37718	-3.38306	1.19663
C	20.58255	-4.11306	1.19663
C	24.63317	-4.96970	1.19663
C	27.15994	-3.71576	1.19663
C	28.31466	-2.87956	1.19663
C	30.42847	-1.00428	1.19663
C	0.55913	0.47014	2.44529
C	1.52843	1.51231	2.44530
C	3.66834	3.38348	2.44529
C	4.87404	4.11302	2.44529
C	8.92486	4.97073	2.44530
C	11.45157	3.71596	2.44529
C	12.60663	2.87963	2.44530
C	14.72039	1.00434	2.44529
C	15.76405	0.03541	2.44529
C	17.73890	-2.02210	2.44529
C	18.79853	-2.96454	2.44530
C	21.22946	-4.44146	2.44529
C	22.47321	-5.06400	2.44530
C	25.27453	-4.73282	2.44530
C	26.56247	-4.09694	2.44529
C	28.85510	-2.44078	2.44529
C	29.91474	-1.49392	2.44530
C	7.47678	5.47269	2.44529
C	23.18515	-5.47235	1.19662
H	7.52417	6.60752	2.44528
H	23.23549	-6.60722	1.19660

LatticeVectors
31.4159 0.0000 0.0000
0.0000 100.0000 0.0000
0.0000 0.0000 2.497322

hydride of **c**

C	0.05122	0.13143	1.29701
C	0.37516	0.77365	0.05183
C	1.08164	2.02703	0.05185
C	1.42239	2.65507	1.29700
C	2.13198	3.90307	1.29700
C	2.46592	4.53399	0.05185
C	3.16836	5.78299	0.05184
C	3.51797	6.40665	1.29701
C	4.36450	7.55816	1.29701
C	4.88028	8.07054	0.05184
C	6.04229	8.90216	0.05190
C	6.71536	9.22201	1.29704
C	8.01828	9.73953	1.29715
C	8.83059	9.92221	0.05204
C	10.00090	8.90413	0.05190

C	10.50050	8.40621	1.29705
C	11.46395	7.32885	1.29704
C	11.88929	6.75396	0.05188
C	12.70390	5.56886	0.05190
C	13.05234	4.94753	1.29706
C	13.76601	3.69868	1.29709
C	14.10416	3.07029	0.05191
C	14.80939	1.81441	0.05193
C	15.13241	1.17327	1.29708
C	15.75962	-0.13103	1.29709
C	16.08266	-0.77239	0.05194
C	16.78950	-2.02707	0.05195
C	17.12970	-2.65413	1.29709
C	17.84040	-3.90342	1.29710
C	18.17348	-4.53228	0.05190
C	18.87721	-5.78263	0.05190
C	19.22351	-6.40271	1.29704
C	20.07523	-7.55635	1.29702
C	20.57901	-8.06362	0.05188
C	21.73801	-8.92691	0.05187
C	22.33595	-9.30092	1.29705
C	23.72829	-9.94847	1.29715
C	24.44653	-9.54404	0.05197
C	25.57210	-8.71822	0.05187
C	26.13605	-8.26514	1.29704
C	27.14321	-7.26204	1.29698
C	27.59919	-6.71809	0.05185
C	28.42304	-5.55952	0.05181
C	28.77304	-4.94104	1.29695
C	29.47761	-3.69587	1.29700
C	29.81561	-3.06710	0.05178
C	30.51757	-1.81289	0.05185
C	30.84057	-1.17035	1.29698
H	9.28696	10.95357	0.05337
H	23.57971	-11.06835	1.29827

LatticeVectors

31.415900	0.000000	0.000000
0.000000	100.000000	0.000000
0.000000	0.000000	2.490319

hydride of **d**

C	0.05449422	0.16445831	1.19152046
C	0.27085254	0.85643762	-0.05180689
C	0.76816093	2.20977711	-0.05181558
C	1.00582182	2.88181471	1.19152054
C	1.50848857	4.23164514	1.19151953
C	1.73694026	4.91748036	-0.05181192
C	2.2396338	6.26554735	-0.05180236
C	2.47531496	6.93820161	1.19151502

C	2.97065376	8.28775488	1.19152404
C	3.18637163	8.9751134	-0.05180896
C	3.62608881	10.33702477	-0.05180035
C	3.90837831	10.99288006	1.19151477
C	4.56168301	12.25777098	1.19151957
C	4.98133237	12.84787413	-0.05180803
C	6.02261136	13.81297681	-0.05180451
C	6.64542669	14.20404422	1.19151902
C	7.93085141	14.74030634	1.19152044
C	8.7467797	14.84513058	-0.05180195
C	9.79106782	13.69583193	-0.0518047
C	10.21803649	13.13904266	1.19151796
C	11.0319072	11.92599572	1.19152062
C	11.36832984	11.29080227	-0.05180634
C	11.99334047	9.97933212	-0.05180065
C	12.29378507	9.322427	1.19151608
C	12.84206819	7.98659266	1.19152751
C	13.13373476	7.33009887	-0.0518091
C	13.65765504	5.98447669	-0.05180381
C	13.89111247	5.30045532	1.1915161
C	14.38655944	3.94353191	1.19152027
C	14.60737034	3.26265702	-0.05180652
C	15.03169332	1.88293193	-0.05180441
C	15.25080751	1.19345503	1.19151966
C	15.74714267	-0.16828732	1.19152002
C	15.9775791	-0.8604877	-0.0518057
C	16.48042477	-2.21863506	-0.051805
C	16.71646715	-2.89594531	1.19151888
C	17.21761246	-4.25503396	1.19151984
C	17.44707285	-4.94584871	-0.05180485
C	17.94693054	-6.30884372	-0.05180584
C	18.17820138	-7.00107454	1.19151892
C	18.70017895	-8.35263491	1.19152166
C	18.9878789	-9.01569287	-0.0518053
C	19.50911753	-10.36372912	-0.05180547
C	19.75100945	-11.04151518	1.19151964
C	20.38061274	-12.34369908	1.19151934
C	20.78340256	-12.94623344	-0.05180708
C	21.79281691	-13.99250284	-0.05180521
C	22.35292559	-14.41230825	1.19152103
C	23.74561678	-15.06541078	1.19151902
C	24.44745086	-14.62835661	-0.05180469
C	25.40884173	-13.60887087	-0.05180439
C	25.90961436	-13.06917868	1.19152111
C	26.74091273	-11.91089498	1.19152201
C	27.08356605	-11.27336949	-0.05180406
C	27.70286529	-9.97128301	-0.05180332
C	28.00431897	-9.31488184	1.19151187
C	28.55109294	-7.98197724	1.19152219
C	28.8428998	-7.32354796	-0.0518129

C 29.3642942 -5.97725112 -0.05182476
C 29.59411195 -5.2881192 1.19149196
C 30.09582503 -3.93480244 1.19151911
C 30.33294644 -3.26103103 -0.05180451
C 30.830247 -1.90597496 -0.05180394
C 31.0463759 -1.21241666 1.19152018
H 9.31915545 15.81578651 -0.05180977
H 23.63032026 -16.18553399 1.19152012
LatticeVectors
31.415900 0.000000 0.000000
0.000000 100.000000 0.000000
0.000000 0.000000 2.486650

hydride of **e**

C 0.06562377 -0.18051173 3.68811491
C 0.24999377 -0.86563043 2.44145612
C 0.58793855 -2.24676287 2.44159804
C 0.77351611 -2.92918717 3.6883573
C 1.10969368 -4.31148308 3.68888693
C 1.29758572 -4.98652217 2.44273917
C 1.63287244 -6.37064089 2.44517356
C 1.82177901 -7.04501752 3.69379915
C 2.15788038 -8.42746527 3.70431824
C 2.34137047 -9.11008929 2.4651743
C 2.68048982 -10.48996026 2.52127173
C 2.87455793 -11.17281657 3.77562133
C 3.29419977 -12.53192147 3.78604488
C 3.51757701 -13.19261483 2.54143003
C 4.01520291 -14.52591346 2.54392667
C 4.24892442 -15.18637501 3.79112343
C 4.77202862 -16.50939995 3.79153564
C 5.07350605 -17.15371139 2.54512994
C 5.72404005 -18.41499006 2.5451287
C 6.12850441 -19.02553356 3.79185886
C 6.9795669 -20.14652427 3.79170916
C 7.69881541 -20.56131933 2.54497084
C 9.04810831 -19.76638199 2.54428219
C 9.57931232 -19.31521573 3.79044613
C 10.49772798 -18.19341019 3.78800981
C 10.82354155 -17.5672191 2.53925367
C 11.27343091 -16.21458661 2.52823371
C 11.4587395 -15.54049625 3.76757572
C 11.79525549 -14.15543929 3.71217646
C 12.00579242 -13.48607103 2.45809822
C 12.49547061 -12.14647356 2.44749123
C 12.70897332 -11.48125295 3.69230193
C 13.05725949 -10.10107516 3.69043415
C 13.2513975 -9.42608995 2.44366596

C	13.66503551	-8.06406601	2.4453089
C	13.86299524	-7.38620341	3.69375526
C	14.20329	-6.00445013	3.70378604
C	14.3896068	-5.3294409	2.46408287
C	14.72387713	-3.94474605	2.5178271
C	14.91193072	-3.26971722	3.77152495
C	15.24906553	-1.88701987	3.78090264
C	15.43469037	-1.20502481	2.53432958
C	15.77271962	0.17646811	2.52514483
C	15.95721024	0.86171522	3.76449757
C	16.2950717	2.24272096	3.71007417
C	16.48102312	2.92342576	2.45632572
C	16.81770976	4.30670432	2.44665092
C	17.00639552	4.98001926	3.69152811
C	17.34236775	6.36418563	3.68928827
C	17.53001685	7.03953798	2.44220745
C	17.86588365	8.42234053	2.44175255
C	18.04945691	9.1054116	3.68828292
C	18.38845117	10.48643888	3.68812402
C	18.5821355	11.16775042	2.44144064
C	19.00145761	12.528428	2.44139462
C	19.22390121	13.18875104	3.68804097
C	19.7220439	14.52339336	3.68804659
C	19.95589474	15.17878842	2.44138096
C	20.48022572	16.50586993	2.44137602
C	20.77625595	17.14115393	3.68802899
C	21.41480596	18.42471625	3.68804017
C	21.74620331	19.02833763	2.4413717
C	22.67491402	20.26409951	2.44137868
C	23.49324597	20.18671085	3.6880377
C	24.76977844	19.63487982	3.68803924
C	25.38109126	19.23538972	2.44137905
C	26.32504451	18.18384714	2.44137871
C	26.6526191	17.55609991	3.68804055
C	27.06542781	16.20264895	3.68804743
C	27.186996	15.51160251	2.44137919
C	27.5008222	14.13118187	2.44138105
C	27.71277218	13.46844159	3.68803801
C	28.20530144	12.13531871	3.6880499
C	28.41786239	11.46778908	2.44137281
C	28.76501487	10.0894445	2.44137839
C	28.96020645	9.4177284	3.6880464
C	29.37342143	8.0566244	3.68803335
C	29.57071516	7.37638647	2.44137869
C	29.91144757	5.99612167	2.44137885
C	30.09683774	5.31954674	3.68803786
C	30.43107343	3.93540416	3.68804718
C	30.619747	3.26264958	2.44137765
C	30.95639065	1.87966944	2.44138452
C	31.14315311	1.20043485	3.68806075

H 7.90921162 -21.66274271 2.54507977
H 22.0421834 21.1932713 2.44137854
LatticeVectors
31.415900 0.000000 0.000000
0.000000 100.000000 0.000000
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