

Supporting information

# First theoretical realization of a stable two-dimensional boron fullerene network

Bohayra Mortazavi

*Department of Mathematics and Physics, Leibniz Universität Hannover, Appelstraße 11,  
30167 Hannover, Germany.*

Corresponding author's email: bohayra.mortazavi@gmail.com

## Atomic structures in VASP POSCAR format

B40-0D-Cage

```
1.0000000000000000
17.0000000000000000 0.0000000000000000 0.0000000000000000
0.0000000000000000 17.0000000000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 17.0000000000000000
```

B

40

Direct

```
0.1330105614824090 0.3959987184940038 0.2576396799855864
0.1371201163535837 0.2353125840353608 0.0665709506697186
0.1520241042248078 0.3754324254076066 0.1636981074810667
0.3375812267318953 0.0745822597380730 0.2576337350537583
0.2352785791860890 0.1371113451764287 0.4040069467094546
0.0795187048450649 0.2352945362327424 0.3510480086874986
0.3743724659547911 0.1835653769035663 0.1361994339766286
0.3754314024773693 0.3185553405734380 0.3069085171535864
0.3376078447892418 0.3959936644138250 0.2576592394120089
0.3334895608354392 0.2353021826703675 0.0665874286140623
0.3185802964154241 0.3754210315866149 0.1637189536450961
0.0745898282279578 0.1330141429772582 0.2129364132565735
0.1520075449605762 0.0951747974003547 0.1636778214994509
0.3185696691786417 0.0951631046050562 0.1636903536373306
0.2870074468764025 0.0962200956142755 0.3343903803008363
0.1835716199709882 0.3743595468324896 0.3343966469432842
0.3743753627475776 0.2870179006529960 0.1362148380512212
0.1835606384741723 0.0962244404343296 0.3343865240064801
0.2352884516033217 0.0795475735345147 0.1195161841063280
0.0745891013584442 0.3376082081838088 0.2129415358748221
0.0962249575443953 0.2870328646214781 0.1361885439351155
0.0962240803917698 0.1835852457033618 0.1361824346352944
0.3754240240068352 0.1519972478366095 0.3068997384006957
0.0951565491061315 0.3185736247366504 0.3068764511193366
0.0951531618966121 0.1520197553734834 0.3068745005522546
0.2875885853302832 0.1527116006643678 0.0856971121279627
0.1830021383092307 0.1527133493078042 0.0856807643271598
0.1329987675476966 0.0746006712981081 0.2576194424490655
0.1526788864874462 0.1830012969782551 0.3848845599649228
0.3910544581645310 0.2352740518421853 0.3510777696190739
0.2870213065306005 0.3743491065286574 0.3344026089724764
0.2875981025056026 0.3178925447663605 0.0857093617197973
0.1830169026932615 0.3179013504664847 0.0856993779692783
0.1526818375314718 0.2875757198756134 0.3848842814191374
0.3959963399008395 0.1329884434595336 0.2129546908389217
0.2353089523943775 0.3910601513263025 0.1195353997942799
0.3178852536739035 0.1829895716706370 0.3849016161707127
0.2352840418012586 0.3334496681034413 0.4040043722732772
0.3960125214366992 0.3375866846651316 0.2129707942115983
0.3178852671704780 0.2875625707201727 0.3848992270230936
```

B40-2D-netwok

1.000000000000000

7.637699999999997

0.000000000000000

0.000000000000000

0.000000000000000

7.637699999999997

0.000000000000000

0.000000000000000

0.000000000000000

20.000000000000000

B

40

Direct

0.3282865740955856	0.9605448433583987	0.5216164626161515
0.3797534530407631	0.5714266762760403	0.3640258531068739
0.3817854988048666	0.8759886305913156	0.4454149656160240
0.8145710534249986	0.1823126758771920	0.5216177242960924
0.5714291902542925	0.3797624241354995	0.6400966889691944
0.1857276706825033	0.5714311453153584	0.6018243331093487
0.8494775044432785	0.4598516436384514	0.4266196246794465
0.8759912350277901	0.7610877566143444	0.5587040670441752
0.8145728512165178	0.9605453508577497	0.5216160892075976
0.7631000050057253	0.5714269432054806	0.3640253711419916
0.7610752361174136	0.8759904722315781	0.4454142112615500
0.1823122607134522	0.3282660598015354	0.4824996097844050
0.3817828331626103	0.2668649100957836	0.4454154894351063
0.7610704807943449	0.2668663498265644	0.4454159938396813
0.6830026534743894	0.2933781573296486	0.5775053214456563
0.4598572459599453	0.8494805389895248	0.5775033107347838
0.8494796777840108	0.6830045369468465	0.4266179501320551
0.4598549817107411	0.2933767628565391	0.5775060630848614
0.5714265663523150	0.1857114758459630	0.4022708407320721
0.1823145050682697	0.8145903943787260	0.4824986265736229
0.2933799071666670	0.6830033945430429	0.4266199877067791
0.2933763394039204	0.4598506049061584	0.4266196652075962
0.8759904547193500	0.3817709558385047	0.5587049437515006
0.2668691750784049	0.7610878257198266	0.5587051851139790
0.2668683106975678	0.3817700580616119	0.5587051991454501
0.6883702181595979	0.3721013044059305	0.3782866121744277
0.4544808834649032	0.3720992125048710	0.3782855531628826
0.3282862412646992	0.1823127348958238	0.5216178612405571
0.3721068285254390	0.4544982675463132	0.6258348753581444
0.9571330918213903	0.5714298544470253	0.6018237184547530
0.6830040033023295	0.8494821159927000	0.5775038107787225
0.6883733300578712	0.7707545066848382	0.3782851572066122
0.4544852834188688	0.7707518169064684	0.3782857240201523
0.3721094087387513	0.6883615458196246	0.6258347075359865
0.9605428719690394	0.3282673972468899	0.4824987736938553
0.5714284893496284	0.9571411975442672	0.4022701181196950
0.7707519329273609	0.4544986694729118	0.6258344471184074
0.5714305008712017	0.7631007073464104	0.6400958462794151
0.9605459040756230	0.8145904910427859	0.4824973977873199
0.7707527088535642	0.6883626669014262	0.6258346063330436