Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

1. Detailed information of relaxed structures

Table 1. The maximum, minimum, and average bond length of six BN-diamondoids with relaxed structures

molecule	Bond length (Å)	B-N bond	B-H bond	N-H bond
$B_4N_6H_{16}$	Maximum	1.595	1.194	1.093
	Minimum	1.516	1.176	1.015
	Average	1.552	1.183	1.056
$B_6N_4H_{16}$	Maximum	1.587	1.257	1.016
	Minimum	1.508	1.185	1.004
	Average	1.537	1.211	1.009
$B_7N_7H_{20}$	Maximum	1.654	1.224	1.059
	Minimum	1.497	1.175	0.971
	Average	1.565	1.200	1.013
$B_8N_{10}H_{24}$	Maximum	1.608	1.220	1.110
	Minimum	1.488	1.168	0.972
	Average	1.556	1.189	1.039
$B_{10}N_8H_{24}$	Maximum	1.625	1.252	1.074
	Minimum	1.498	1.145	0.972
	Average	1.541	1.200	1.030
$B_{11}N_{11}H_{28}$	Maximum	1.663	1.198	1.063
	Minimum	1.487	1.152	1.009
	Average	1.554	1.178	1.044

The structural models of six BN-diamondoids in the XYZ file format are provided as follow.

$B_4N_6H_{16}$ structure:

26
final(relaxed) structure
N 1.32679 0.04969 0.68654
N -0.79997 -1.22254 0.59308
N -0.80170 1.22547 0.59225
N 0.68252 -1.22291 -1.42229
N -1.54097 -0.04422 -1.42662
N 0.68183 1.22575 -1.42433
B -0.10732 0.01497 1.24804
B 1.43490 0.01535 -0.87485
B -0.82893 -1.28862 -0.93530
B -0.83762 1.27222 -0.94132
H -0.11056 0.00241 2.44233
H 1.89908 0.84601 1.06273

H 1.79852 -0.84340 0.96171
H -1.79044 -1.26747 1.05278
H -0.32266 -2.10785 0.95494
H -1.79078 1.27230 1.05247
H -0.32374 2.11247 0.95394
H 2.54698 0.00232 -1.26482
H -1.38021 -2.23035 -1.37251
H -1.38119 2.23035 -1.37279
H 0.63770 -1.26755 -2.43880
H 1.15870 -2.10837 -1.05845
H -1.59200 0.00024 -2.43974
H -2.53685 -0.00024 -1.05676
H 0.63757 1.27260 -2.43912
H 1.15706 2.11295 -1.05877

$B_6N_4H_{16}$ structure:

26
final(relaxed) structure
B 1.56650 0.01201 0.93846
B -0.61748 -1.27756 0.86884
B -0.55051 1.24118 0.86079
B 0.83408 -1.20244 -1.20142
B -1.30664 -0.00227 -1.21235
B 0.84924 1.28437 -1.23090
N 0.05802 -0.04999 1.42683
N 1.53839 0.04783 -0.58504
N -0.58378 -1.21916 -0.68163
N -0.58277 1.21737 -0.68499
H 0.10209 -0.00299 2.43667
H 2.12297 0.96031 1.38004
H 2.12041 -0.95927 1.38022
H -1.70675 -1.27512 1.37613
H -0.10301 -2.23486 1.37607
H -1.69675 1.27269 1.37585
H -0.10294 2.23158 1.37712
H 2.44008 0.00171 -1.05031
H -1.06072 -2.01829 -1.05864
H -1.06181 2.01762 -1.05690
H 0.84849 -1.27063 -2.43511
H 1.38305 -2.22961 -0.84535

H -1.37795 -0.00003 -2.43774
H -2.44816 -0.00188 -0.84545
H 0.84727 1.27173 -2.43729
H 1.38336 2.23121 -0.74153

$B_7N_7H_{20}$ structure:

34
final(relaxed) structure
B -0.08310 0.00922 2.29624
B 1.37600 0.00407 0.09739
B -0.84250 -1.29426 0.08425
B -0.85384 1.25895 0.06580
B 0.72903 -1.29109 -2.02087
B -1.53768 -0.01118 -2.03485
B 0.71992 1.26489 -2.02650
N 1.33030 0.05004 1.74117
N -0.78653 -1.22468 1.64569
N -0.78865 1.22308 1.64258
N 0.58961 -1.22103 -0.37608
N -1.52735 -0.04706 -0.38102
N 0.58818 1.21952 -0.37814
N -0.04881 -0.04652 -2.48813
H -0.10576 -0.00020 3.49633
H 1.90544 0.84751 2.01276
H 1.90699 -0.74269 2.01345
H -1.70510 -1.27339 2.01510
H -0.32243 -2.10599 2.00587
H -1.70521 1.27483 2.01506
H -0.32074 2.11117 1.90565
H 2.54367 -0.00028 -0.21166
H -1.48132 -2.23350 -0.21450
H -1.48121 2.22812 -0.21503
H 1.16336 -2.01621 -0.10723
H -2.45728 -0.00138 -0.10395
H 1.16226 2.01587 -0.10786
H 1.90784 -1.27077 -2.32768
H 0.10908 -2.23078 -2.43329
H -2.11809 -0.96211 -2.43508
H -2.11529 0.95869 -2.43346
H 1.90623 1.26921 -2.32772

H 0.10929 2.22571 -2.43423
H -0.00020 -0.00201 -3.49709

$B_8N_{10}H_{24}$ structure:

42
final(relaxed) structure
B -0.74310 0.01052 2.27084
B 0.67992 0.00520 0.12623
B -1.53993 -1.26175 0.08724
B -1.52102 1.28148 0.10865
B -0.05629 -1.28301 -1.98472
B -2.28748 0.00696 -1.98595
B -0.10872 1.25799 -1.98569
B 2.20519 0.00467 -1.96680
N 0.68997 0.04874 1.64610
N -1.52315 -1.22260 1.64415
N -1.52320 1.22338 1.64663
N 2.07993 -0.04595 -0.37536
N -0.05370 -1.22231 -0.37768
N -2.26240 0.04833 -0.37912
N -0.05326 1.22316 -0.37917
N 1.43156 -1.22491 -2.48384
N 1.33475 1.22224 -2.48370
N -0.79268 -0.04647 -2.48451
H -0.73445 0.00043 3.49123
H 1.27425 0.84448 2.01026
H 1.17301 -0.84467 1.91080
H -2.44316 -1.26979 2.01761
H -1.05699 -2.10772 2.00754
H -2.44356 1.27112 2.01696
H -1.05734 2.10862 2.00830
H 2.64302 0.83488 -0.00292
H 2.64790 -0.84640 0.00014
H 3.29476 0.00283 -2.43101
H 1.38678 -1.27135 -3.49780
H 1.90749 -2.10773 -2.12299
H 1.38306 1.27165 -3.49740
H 1.80214 2.10919 -2.12178
H -2.11175 -2.22663 -0.31610
H -2.11294 2.23470 -0.21462

H 0.42812 -2.11233 -0.10199
H -3.19228 0.00158 -0.09893
H 0.42898 2.11317 -0.10362
H -0.62736 -2.22950 -2.43146
H -2.85574 -0.96196 -2.32948
H -2.85160 0.95913 -2.43353
H -0.63217 2.22786 -2.43177
H -0.84107 -0.00149 -3.49616

$B_{10}N_8H_{24}$ structure:

42
final(relaxed) structure
N -0.78295 -0.04626 2.38885
N 0.79646 0.05012 0.37433
N -1.33476 -1.22128 0.37369
N -1.33507 1.22183 0.37254
N 0.05498 -1.22287 -1.73807
N -2.07569 -0.04427 -1.73558
N 0.05296 1.22412 -1.73847
N 2.26299 -0.04706 -1.73458
B 0.68963 -0.00276 1.90523
B -1.46432 -1.29915 1.93218
B -1.41681 1.26282 1.92798
B 2.21062 0.00617 -0.18243
B 0.08128 -1.26388 -0.13416
B -2.13064 -0.00336 -0.11173
B 0.07861 1.28497 -0.15133
B 1.51839 -1.28474 -2.20568
B 1.52939 1.25487 -2.16384
B -0.66864 -0.00344 -2.26045
H -0.64393 -0.00107 3.39405
H 1.37204 0.95318 2.33832
H 1.37276 -0.95104 2.33929
H -2.56074 -1.27232 2.33538
H -0.84712 -2.23162 2.33635
H -2.55130 1.27496 2.33479
H -0.84617 2.23109 2.33815
H 2.86020 0.95729 0.22093
H 2.85952 -0.95403 0.22225
H 3.19277 0.00023 -2.01377

H 1.58381 -1.27253 -3.39485
H 2.11587 -2.23190 -1.79298
H 1.58582 1.27464 -3.38858
H 2.11686 2.23159 -1.79266
H -1.90230 -2.00982 0.00982
H -1.90322 2.01188 0.01168
H 0.63710 -2.22956 0.21954
H -3.28619 0.00151 0.21759
H 0.63675 2.23592 0.21838
H -0.42106 -2.10853 -2.00649
H -2.64760 -0.84422 -2.00948
H -2.64137 0.82715 -2.00616
H -0.42034 2.11101 -2.00787
H -0.74257 0.00130 -3.40294

$B_{11}N_{11}H_{28}$ structure:

50
final(relaxed) structure
B -0.83466 -0.00475 3.28131
B 0.61248 -0.00943 1.14173
B -1.60381 -1.25607 1.11498
B -1.59491 1.28613 1.13426
B 2.13555 -0.00316 -0.97553
B -0.12473 -1.22638 -0.97718
B -2.32964 0.02141 -0.95538
B -0.11353 1.25995 -0.96688
B -0.87482 0.00027 -2.98373
B 1.38693 -1.28682 -3.01887
B 1.37918 1.26341 -3.02618
N 0.58727 -0.04326 2.70094
N -1.54210 -1.22364 2.70223
N -1.54052 1.22438 2.70310
N 2.06670 -0.04348 0.68551
N -0.15223 -1.22404 0.68350
N -2.28184 0.04612 0.68525
N -0.15023 1.22450 0.68540
N 1.33055 -1.22189 -1.42638
N 1.33114 1.22219 -1.42565
N -0.89172 0.04834 -1.42608
N 0.58889 -0.04632 -3.44538

H -0.83991 0.00046 4.45342
H 1.06176 0.83190 3.06484
H 1.06915 -0.84919 3.07025
H -2.52648 -1.26907 3.06304
H -1.15963 -2.11319 3.06446
H -2.52570 1.26951 3.06314
H -1.15933 2.11385 3.06553
H 2.54280 0.83158 1.04993
H 2.55092 -0.84919 1.05580
H 3.29079 0.00048 -1.27253
H 1.79849 -2.10492 -1.07005
H 1.79947 2.10615 -1.07083
H 2.54992 -1.27044 -3.28904
H 0.74458 -2.23388 -3.28927
H 2.54835 1.27032 -3.28935
H 0.74434 2.23001 -3.28994
H -2.21909 -2.22835 0.84033
H -2.21837 2.23410 0.84105
H 0.31635 -2.10646 1.04588
H -3.26704 0.00272 1.04644
H 0.31745 2.10710 1.04669
H -0.63666 -2.23165 -1.27561
H -2.86051 -0.96444 -1.27487
H -2.96243 0.96206 -1.27521
H -0.63692 2.23852 -1.27503
H -1.48061 -0.96171 -3.28903
H -1.47912 0.96260 -3.29201
H 0.53657 -0.00136 -4.45250

2. Comparison between the density of states of BN-diamondoids and the corresponding carbon-based diamondoids

The density of states is calculated in DFT level with small gaussian smearing of 0.03 eV spreading. The energies of highest occupied states are shifted to zero.

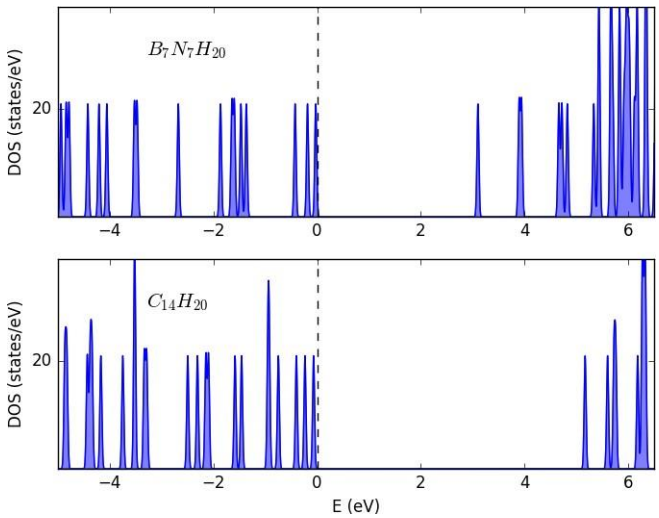

Figure 1. Comparison between the density of states of BN-diamantane and diamantane

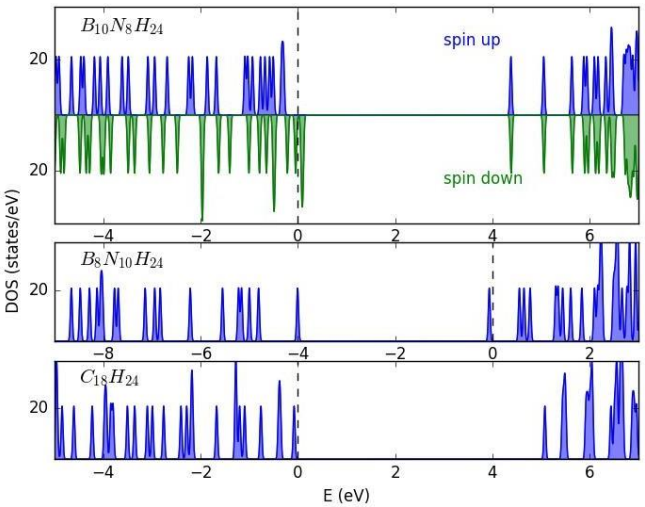

Figure 2. Comparison between the density of states of BN-triamantane, BN-triamantane-iso, and triamantane

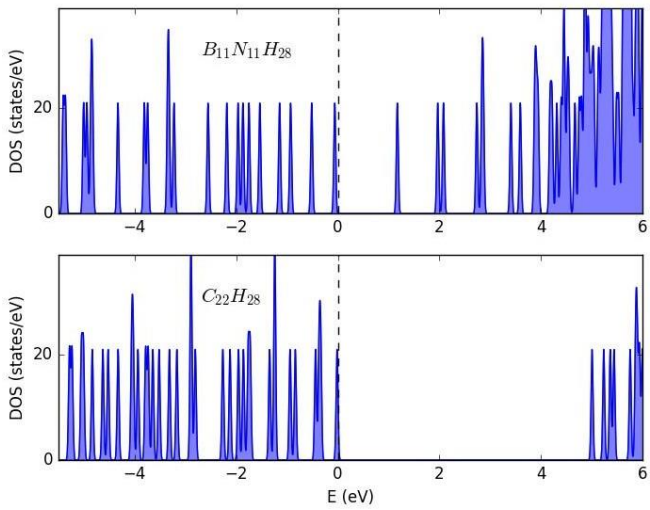

Figure 3. Comparison between the density of states of BN-tetramantane and tetramantane