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Boron aggregation in the ground states of boron-carbon fullerenes

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We present novel structural motifs for boron-carbon nano-cages of the stoichiometries $B_{12}C_{48}$ and $B_{12}C_{50}$, based on first principle calculations. These configurations are distinct from those proposed so far by the fact that the boron atoms are not isolated and distributed over the entire surface of the cages, but rather aggregate at one location to form a patch. Our putative ground state of $B_{12}C_{48}$ is 1.8 eV lower in energy than the previously proposed ground state and violates all the suggested empirical rules for constructing low energy fullerenes. The $B_{12}C_{50}$ configuration is energetically even more favorable than $B_{12}C_{48}$, showing that structures derived from the C_{60} Buckminsterfullerene are not necessarily magic sizes for heterofullerenes.

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Since its discovery by Kroto *et al.* in 1985 [1], the C_{60} fullerene has found a wide range of applications as a building block in the field of nano-science. For instance it is possible to directly form solids out of it [2] or to dope it by adding substitutional or endohedral atoms, e.g. in the context of hydrogen storage [3].

For future applications it would be advantageous to have more such basic building blocks. One possibility is to modify the original carbon fullerene by substitutional doping. A very popular choice for the dopant atoms are boron and nitrogen since they are neighbors to carbon in the periodic table. Various boron-carbon heterofullerenes have been observed experimentally [4, 5]. The existence of cross-linked $N_{12}C_{48}$ fullerenes could explain experimental measurements of thin solid films [6]. The case of boron is of particular importance as it is the p-type counterpart of the n-type nitrogen doping in fullerene and graphene used to tune their electronic or catalytic properties [7, 8].

In order to determine the energetically most favorable structure, it is in principle necessary to perform a numerically costly unbiased global structure search, which became possible only very recently [9–12].

Previous work on heterofullerene cages was therefore based on biased searches that constrained the exploration of the energy landscape to certain structural motifs. For the stoichiometries B_nC_{60-n} this constraint typically consisted in starting the search from the perfect C_{60} fullerene and substituting n carbon atoms by boron. Garg *et al.* [13] extensively investigated the geometries B_nC_{60-n} for $n = 1 - 12$. They concluded that the boron is arranged such that a pentagon ring does not contain more than one and a hexagon not more than two boron atoms (at non-adjacent sites). Putting more boron atoms in a ring increases the bond lengths and decreases the stability. A study by Viani and Santos [14] on various smaller fullerenes again confirmed that boron atoms are

most preferably situated at opposite sites in a hexagon, thereby increasing the bond lengths in their neighborhood. For the heterofullerene $B_{12}C_{48}$, which will be one of the two stoichiometries investigated in this paper, Manaa *et al.* [15] performed a detailed study; they claimed that the best structure was the same that was previously found for $N_{12}C_{48}$ [16], thereby again confirming the previous results stating that the boron atoms should be spread over the entire carbon cage and isolated. We will refer to this class of structures as “diluted”.

We reinvestigated the boron-carbon heterofullerenes by performing for the first time a systematic and unbiased search for low energy minima for the stoichiometries $B_{12}C_{48}$ and $B_{12}C_{50}$.

The Minima Hopping Method (MHM) [12] was used for our unbiased search of new configurations. All calculations were done at the level of Density Functional Theory, using the BigDFT package [17]. This code uses Daubechies wavelets [18] as basis set and HGH pseudopotentials [19] to simulate the core electrons. The exchange correlation part was described by the PBE functional [20], which has shown to give highly reliable energy differences between different structural motifs in boron [21] and is therefore used [22] in this work. Convergence parameters in BigDFT were set such that total energy differences were converged up to 10^{-5} Ha and all configurations were relaxed until the maximal force component on any atom reached the noise level of the calculation, which was of the order of 1 meV/Å.

In order to speed up our exhaustive configurational search we started both from diluted and aggregated configurations with a wide structural diversity, based on various C_n backbones (with $n=60, 58$ or 48). For aggregated configurations we considered both filled hexagons and filled pentagons as they were demonstrated to be building blocks [23, 24] in the B_{80} boron fullerene [25]; furthermore we have inserted compact boron icosaha-

83 drons in opened C_{60} fullerenes. In addition we generated
 84 structures of high symmetry for the stoichiometry C_{48}
 85 and added 12 boron atoms at locations where it seemed
 86 appropriate by intuition. Some short MHM runs start-
 87 ing from the energetically most promising configurations
 88 allowed us to see trends leading to an energy lowering.
 89 From these ones a second set was derived by applying
 90 additional modifications (e.g. exchanging boron and carbon
 91 atoms) in order to speed up the exploration in a second
 92 step of MHM. Finally we systematically exchanged boron
 93 and carbon atoms up to second-nearest neighbors for the
 94 most favorable structures emerging from this process. In
 95 this way we could generate more than thousand configu-
 96 rations containing a large variety of structural motifs.

97 Among our $B_{12}C_{48}$ structures obtained in this way we
 98 found several being considerably lower in energy than the
 99 three most favorable ones identified by Manaa *et al.* [15].
 100 Whereas the new configurations agree with them in the
 101 overall shape exhibiting a cage-like structure, they differ
 102 substantially by the fact that the boron is not distributed
 103 over the entire cluster, but aggregated in a patch, thereby
 104 separating the surface of the compound in a boron-rich
 105 and a boron-poor part. This is in strong contrast to the
 106 widely accepted belief that the boron atoms should be
 107 isolated [26], i.e. be always separated by one or several
 108 carbon atoms. We will refer to our novel structural motif
 109 as “patched”.

110 The low energy part of the spectrum that we have ex-
 111 plored is shown in Fig. 1, together with the structures
 112 of the 12 lowest isomers that we have found, the lowest
 113 structure exhibiting a filled pentagon and the three most
 114 favorable diluted structures. The latter ones turned out
 115 to be identical to the three lowest structures identified
 116 by Manaa *et al.* In total we found 143 new structures
 117 that are lower in energy than the putative ground state
 118 proposed so far. We made however no effort to find all
 119 the structures in this energy interval and so more than
 120 143 structures are expected to exist. The energy levels
 121 are colored on a scale from 0 to 1 which describes the
 122 relative amount of carbon atoms being first neighbors to
 123 boron. Thus a value of 0 (red) means that the boron
 124 atoms are only surrounded by boron – which can obvi-
 125 ously not happen –, whereas a value of 1 (blue) means
 126 that the boron atoms are only surrounded by carbon.
 127 Consequently the coloring of the patched structures tends
 128 towards red values, while the coloring of the diluted ones
 129 tends towards blue values. In the lowest structures the
 130 boron atoms form a patch with frayed boundaries, which
 131 results in astonishing configurations where carbon atoms
 132 have four boron atoms as first neighbors. Furthermore
 133 it is surprising that the lowest structure exhibits a hepta-
 134 gon, which is usually less favorable than the penta- and
 135 hexagons, and twice two adjacent pentagons, which is in
 136 general very disadvantageous [27]. However these pen-
 137 tagons do not only consist of carbon, but there are some
 138 substitutional boron atoms contained within them.

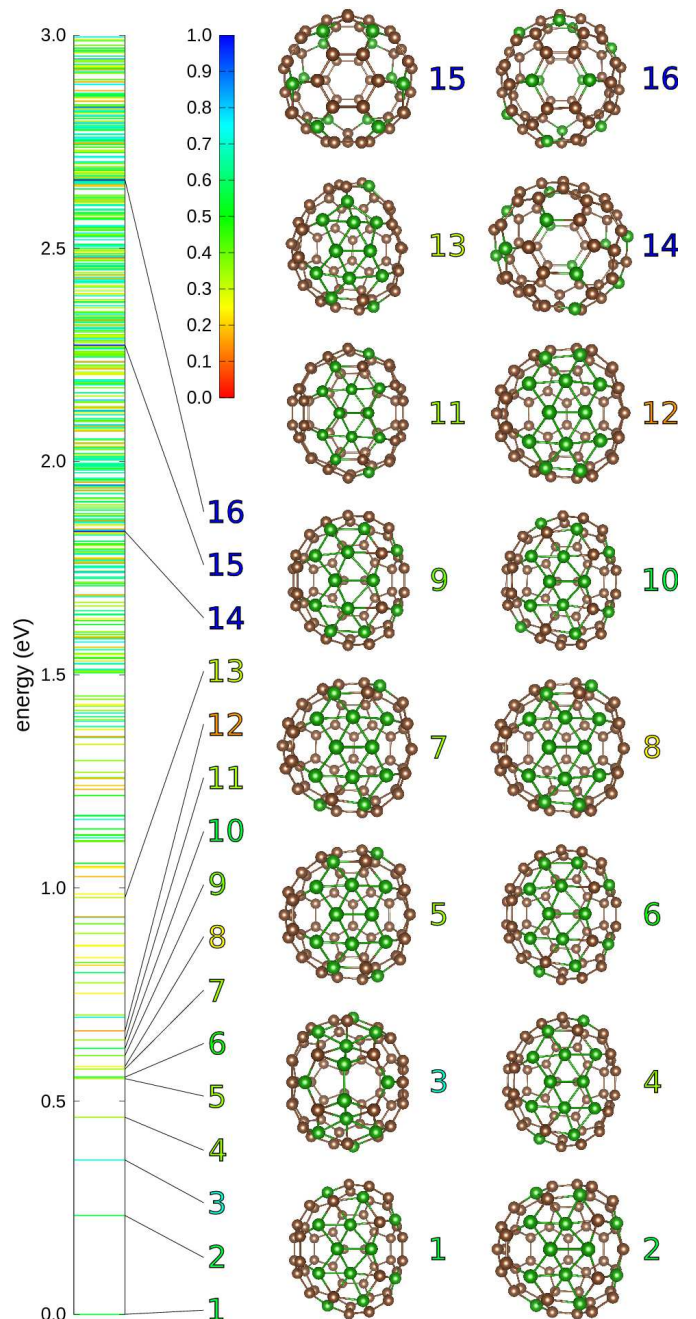


FIG. 1. Plot of the 12 energetically most favorable structures, the most favorable one containing a filled heptagon and the three lowest diluted configurations for $B_{12}C_{48}$, together with the low energy part of the spectrum. The coloring scheme is explained in the text.

139 Tab. I gives some more information about the struc-
 140 tures shown in Fig. 1. The first column shows the en-
 141 ergy separation ΔE of the configurations with respect to
 142 the lowest structure. We can see that our new ground
 143 state is 1.8eV lower in energy than the putative ground
 144 state proposed so far. In the second column we present
 145 the HOMO-LUMO gaps of the structures. The values

	ΔE (eV)	gap (eV)	ΔH (eV)	PG	RMSD (bohr)
1st	0.000	0.457	0.340	C _s	0.000
2nd	0.232	0.477	0.344	C _s	1.003
3rd	0.362	0.646	0.346	C _s	1.717
4th	0.462	0.645	0.348	C ₁	1.092
5th	0.553	0.295	0.350	C _s	1.589
6th	0.557	0.236	0.350	C ₁	0.558
7th	0.575	0.247	0.350	C ₁	1.486
8th	0.582	0.452	0.350	C ₁	1.579
9th	0.607	0.604	0.350	C _s	0.783
10th	0.624	0.378	0.351	C ₁	0.533
11th	0.644	0.616	0.351	C _s	1.344
12th	0.665	0.644	0.351	C _s	1.490
27th	0.978	0.695	0.357	C ₁	1.678
144th	1.836	0.494	0.371	S ₆	3.465
295th	2.273	0.316	0.378	D _{3d}	3.501
453th	2.661	0.302	0.385	S ₆	3.442

TABLE I. Properties of the structures shown in Fig. 1.

range from 0.2 eV to 0.7 eV, thus being rather small, and do not exhibit any special pattern. In particular there is no notable difference between the class of the patched and the diluted structures. The next column shows the formation energies per atom ΔH with respect to the bulk conformations of boron and carbon (α -boron and cubic diamond, respectively), which is defined by $\Delta H = (E - n_B E_B^0 - n_C E_C^0)/(n_B + n_C)$ with E being the energy of the compound and E_X^0 and n_X being the energy per atom of the reference configurations and the number of atoms, respectively. In the next column we give the point groups of the structures. Whereas the diluted structures are rather symmetric (point groups S₆ and D_{3d}), the new structures are of much lower symmetry (C_s and C₁). Finally we present the RMSD [28] of the structures with respect to the new putative ground state. It is obvious that there is a clear separation between the patched structures and the diluted ones. Within the patched ones, however, there is no relation between the energy and the RMSD.

A more complete overview of the energies and the corresponding RMSD values is shown in Fig. 2(a). Here we plot for all structures up to 8 eV the energy difference and the RMSD with respect to the putative ground state. As can be seen there is a broad range with structures whose energies are completely uncorrelated to the value of the RMSD. However this range is sharply bounded at a value of about 2 bohr, separating it from energetically higher configurations.

By filling the heptagon in the putative ground state of B₁₂C₄₈ by two carbon atoms – thus modifying it into a pentagon and a hexagon – the two adjacent pentagons which are present twice on both sides of the heptagon are turned into a pentagon and a hexagon each. Since this structure consists only of pentagons and hexagons and furthermore respects the isolated pentagon rule, it

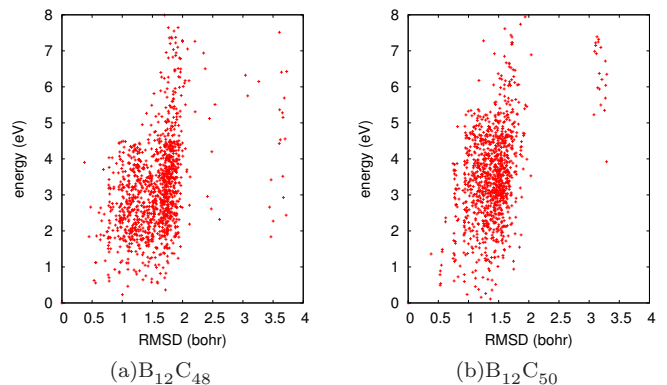


FIG. 2. The energy difference versus the RMSD, both with respect to the putative ground states.

is a promising candidate for the global minimum of the stoichiometry B₁₂C₅₀.

In order to confirm this assumption we again performed an extended and unbiased search for the ground state. We again used several approaches to generate many different input structures: We added two atoms to the lowest isomers of B₁₂C₄₈ as described; we replaced ten carbon atoms by boron in a C₆₀ and added two additional interstitial boron atoms at appropriate positions; and we replaced 12 carbon atoms by boron starting from a C₆₂ fullerene. For this last approach we took two examples that were first described by Ayuela *et al.* [29] and Qian *et al.* [30] and turned out to be the most stable C₆₂ isomers in a study by Cui *et al.* [31]. As for the case of B₁₂C₄₈ we again continued by either manually rearranging the atoms or by using the configurations as input for subsequent MHM runs.

It turned out that the structure that we constructed by hand from the ground state of B₁₂C₄₈ is energetically the most favorable one. In addition, at least 673 patched structures are lower in energy than the most favorable diluted configuration which is 3.9 eV higher in energy than our ground state. The low energy part of the spectrum is shown in Fig. 3, together with figures of the 12 structures being lowest in energy, the most favorable one containing a filled pentagon and the two most favorable diluted configurations. The energy levels are coded in colors in analogy to Fig. 1. As for the case of B₁₂C₄₈ it is clear that all low lying minima correspond to the same structural motif where the boron is aggregated in a patch.

In Tab. II we present some more information about the structures shown in Fig. 3. The HOMO-LUMO gaps are – except for the few lowest structures – in general smaller than the ones for B₁₂C₄₈; again there is no notable difference between the patched and the diluted structures. The values for the formation energy ΔH are slightly lower than their counterparts for B₁₂C₄₈ in Tab. I, indicating that it is more likely to encounter experimen-

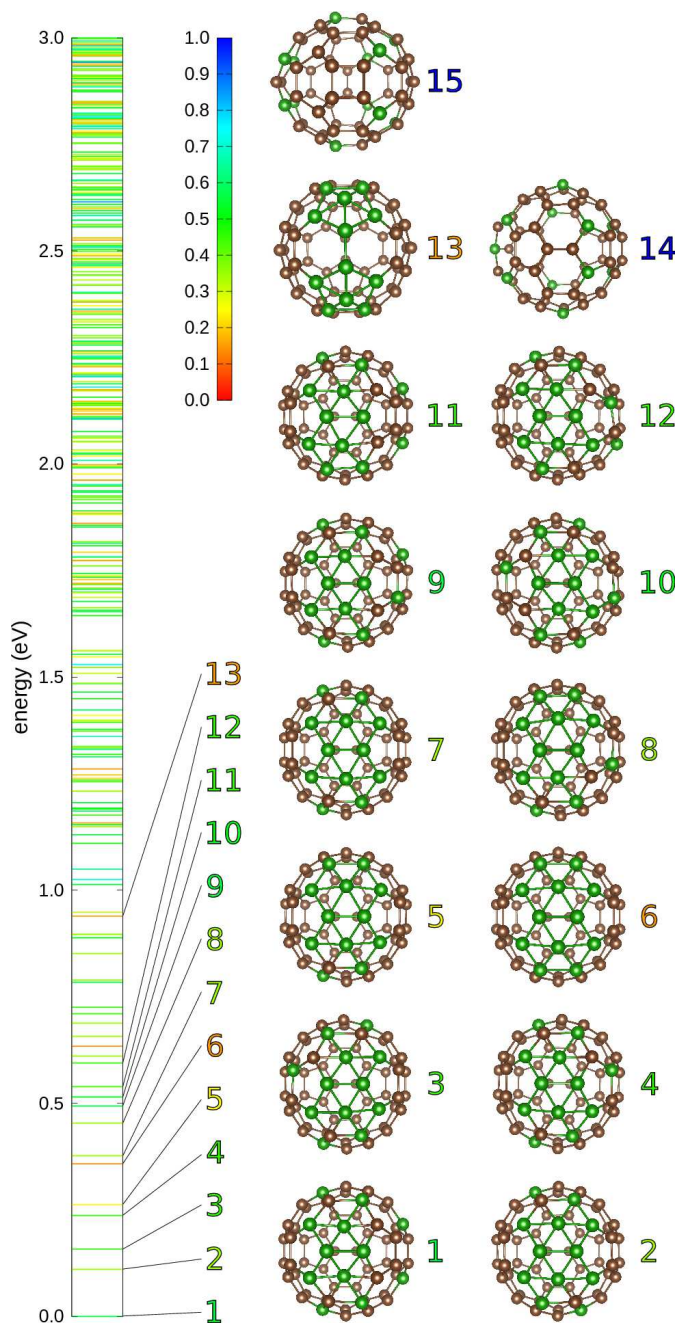


FIG. 3. The low energy part of the spectrum for $B_{12}C_{50}$, together with figures of the 12 energetically lowest structures, the most favorable one containing a filled pentagon and the two most favorable diluted configurations.

222 tally the stoichiometry $B_{12}C_{50}$ than $B_{12}C_{48}$. The point
 223 groups exhibit a wider variation compared to the case of
 224 $B_{12}C_{48}$; the energetically most favorable structures have
 225 the point groups C_1 , C_2 , C_s and C_{2v} . On the other hand
 226 the diluted structures are of lower symmetry than their
 227 counterparts for $B_{12}C_{48}$ and exhibit only the point group
 228 C_s . The RMSD behaves similar as for $B_{12}C_{48}$. A more
 229 complete overview of the energy versus the RMSD – anal-

	ΔE (eV)	gap (eV)	ΔH (eV)	PG	RMSD (bohr)
1st	0.000	0.534	0.322	C_s	0.000
2nd	0.110	0.416	0.324	C_2	1.363
3rd	0.158	0.434	0.325	C_1	1.209
4th	0.237	0.283	0.326	C_1	0.976
5th	0.262	0.338	0.327	C_1	1.285
6th	0.358	0.308	0.328	C_{2v}	1.390
7th	0.377	0.154	0.328	C_s	1.168
8th	0.453	0.215	0.330	C_1	1.113
9th	0.494	0.249	0.330	C_1	0.530
10th	0.515	0.380	0.331	C_1	1.451
11th	0.539	0.227	0.331	C_1	0.539
12th	0.595	0.363	0.332	C_1	0.931
25th	0.939	0.296	0.337	C_{2v}	1.750
673th	3.921	0.204	0.386	C_s	3.289
965th	5.227	0.458	0.407	C_s	3.080

TABLE II. The same data as in Tab. I, this time for the structures shown in Fig. 3.

230 ogous to the one shown in Fig. 2(a) – is given in Fig. 2(b).
 231 Both the last column of Tab. II and Fig. 2(a) show again
 232 a clear separation between the patched and the diluted
 233 configurations.

234 In conclusion, we have shown that the ground state of
 235 boron-carbon heterofullerenes is fundamentally different
 236 from what was thought previously. It consists of incom-
 237 plete carbon cages whose openings are filled with boron
 238 patches. In a broader context our results show that
 239 doping in sp^2 -materials is not yet well understood and
 240 that no universally valid rules are available to predict
 241 which structural motifs are the most stable ones in such
 242 doped structures. Our results could also give guidance
 243 to synthesis efforts [32] for such heterofullerenes. The
 244 step rise of the energy of metastable configurations
 245 as a function of the distance from the ground state
 246 shown in Fig. 2 indicates that there is a substantial
 247 driving force towards low energy motifs with patches and
 248 suggests that a synthesis of patched structures should
 249 be possible. The energy gap between the ground state
 250 and the lowest metastable state (0.2 eV for $B_{12}C_{48}$ and
 251 0.1 eV for $B_{12}C_{50}$) is however much smaller than in C_{60}
 252 (1.6 eV) and reaching the ground state might therefore
 253 be difficult. The standard synthesis procedure of substi-
 254 tuting [5] carbon atoms by boron atoms is unlikely to
 255 succeed for heterofullerenes containing a larger number
 256 of boron atoms which then form patches. Planar boron
 257 clusters that are structurally similar to the boron patches
 258 found in our ground state can however be synthesized ex-
 259 perimentally [33] and might form growth nuclei for such
 260 heterofullerenes in a carbon rich spark or vapor chamber.

261
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