STUDIA UBB CHEMIA, LXI, 1, 2016 (p. 283-290)
(RECOMMENDED CITATION)

Dedicated to Professor Mircea Diudea on the Occasion of His 65th Anniversary

ON BIPARTITE EDGE FRUSTRATION OF CARBON AND BORON NANOTUBES

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ABSTRACT. The measure of bipartivity is one of the important topological and structural property which describes the chemical stability of underlying chemical structures. Bipartite edge frustration is one of the topological descriptors which calculate measure of bipartivity of a chemical structure. Carbon hexagonal nanotubes, boron triangular nanotubes and boron α-nanotubes are important nanostructures, which have been studied extensively by both of the theoretical and computational chemists. In this article, we consider carbon hexagonal nanotubes, boron triangular nanotubes and boron α-nanotubes for the study of bipartite edge frustration.

Keywords: *Bipartite edge frustration, Carbon hexagonal nanotube, Boron triangular nanotube, Boron α-nanotube*

INTRODUCTION

Nanotechnology works with structures of size in the range 1 to 100 nanometers. Nanotechnology creates many new materials and devices with a variety of applications in medicine, electronics, and computer. The most significant nano structures are carbon nanotubes, boron triangular nanotubes and boron α-nanotubes (Figure 1).

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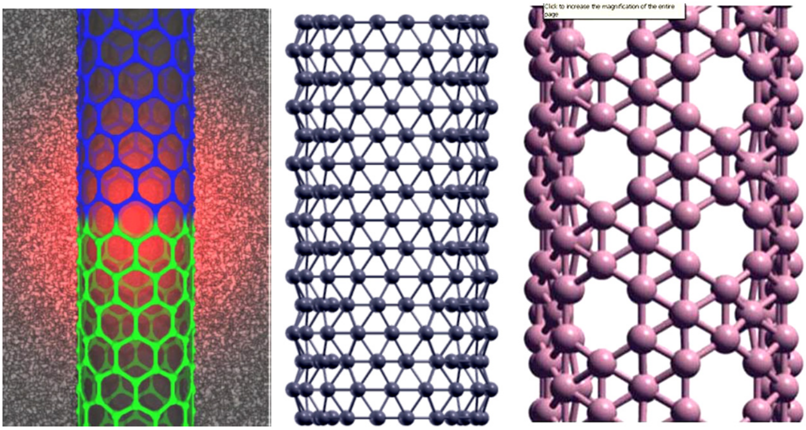
The recent discovery of pure boron triangular nanotubes challenges the monopoly of carbon. The first boron triangular nanotubes were created in 2004 and consist of triangular sheets [1,2]. Figure 1b shows a boron triangular sheet.

Let $G=(V,E)$ be a simple graph, a graph without multiple edges and loops. A subgraph H of G is a graph whose set of vertices and set of edges are all subsets of G. A spanning subgraph is a subgraph that contains all the vertices of the original graph.



(a) (b) (c)

Figure 1. Carbon hexagonal nanotube (a); Boron triangular nanotube (b); Boron α-nanotube (c).

The graph G is called bipartite if the vertex set V can be partitioned into two disjoint subsets V_1 and V_2 such that all edges of G have one endpoint in V_1 and the other in V_2. Bipartite edge frustration of a graph G denoted by $\phi(G)$, is the minimum number of edges that need to be deleted to obtain a bipartite spanning subgraph.

It is easy to see that $\phi(G)$ is a topological index and G is bipartite if and only if $\phi(G) = 0$. Thus $\phi(G)$ is a measure of bipartivity. It is well-known that a graph G is bipartite if and only if it does not have odd cycles. Holme *et al*. introduced the edge frustration as a measure in the context of complex network [3].

Fajtlowicz claimed that the chemical stability of fullerenes is related to the minimum number of vertices/edges that need to be deleted to make a fullerene graph bipartite [4,5]. However, Schmalz et al. [6] observed that the isolated pentagon fullerenes (IPR fullerenes) have the best stability. Doslic [7] presented some computational results to confirm this relationship. So it is natural to ask about relationship between the degree of non-bipartivity and stability of chemical structures such as nanotubes.

Throughout this paper all the considered graphs are finite and simple. Our notation is standard and taken mainly from [8,9]. We encourage the reader to consult papers by Doslic [7,10,11] for background material and more information on the problem. Also, the reader is referred to papers [12-15] for some background material as well as basic computational methods on mathematical properties of nanomaterials and chemical networks.

RESULTS AND DISCUSSON

Bipartite edge frustration is probably related to the chemical stability of nanostructures, like fullerenes or nanotubes.

Ashrafi *et al*. [16] computed the bipartite edge frustration of various families of carbon nanotubes. Doslic *et a*l. [2,10] studied the bipartite edge frustration of fullerenes. In this paper, the bipartite edge frustration of carbon and boron nanotubes is studied.

Carbon Polyhex Nanotubes

There are different shapes of carbon polyhes nanotubes CNT, such as armchair, chiral and zigzag [2] based on the rolling of 2D carbon polyhex sheet. A CNT of order $n\times m$ is a tube obtained from a carbon polyhexl sheet of n rows and m columns by merging the vertices of last column with the respective vertices of first column (Figure 2).

A zig-zag CNT is a nanotube of order $n\times m$ in which carbon atoms are arranged in zig-zag pattern (Figure 2a). Similarly, an armchair carbon hexagonal nanotube is a carbon nanotube in which carbon atoms are arranged in an armchair pattern (Figure 2b). It can easily be seen that a carbon hexagonal nanotube has only odd number of rows and even number of columns.

A complete regular hexagon with six vertices is called full-hexagon. An incomplete hexagon with four vertices is called a half-hexagon. The first row (last row) of an armchair CNT of order $n\times m$ has *m*/2 number of half-hexagons. For the sake of simplicity we denote zig-zag carbon hexagonal nanotube with CNT_1 and armchair carbon hexagonal nanotube with CNT_2. In a CNT of order $n\times m$, there are $m(n-2)/2$ full hexagons and m half hexagons. The number of vertices and edges in such a CNT are nm and $m(3n-2)/2$ respectively.

In the following, we prove that both of these carbon hexagonal nanotubes have zero bipartite edge frustration.

Theorem 2.1.1. Let CNT_1 and CNT_2 be the zig-zag and armchair carbon hexagonal nanotubes respectively, then

$$\phi(CNT_1) = \phi(CNT_2) = 0$$

Proof. A graph G is bipartite if and only if $\phi(G) = 0$, thus, it suffices to prove them bipartite. Figure 2 shows a 2-coloring of CNT_1, in which bold vertices can be put in one partition and rest of them in the other partition. This clearly shows that CNT_1 is bipartite. Similarly, the bipartivity is proven for CNT_2.

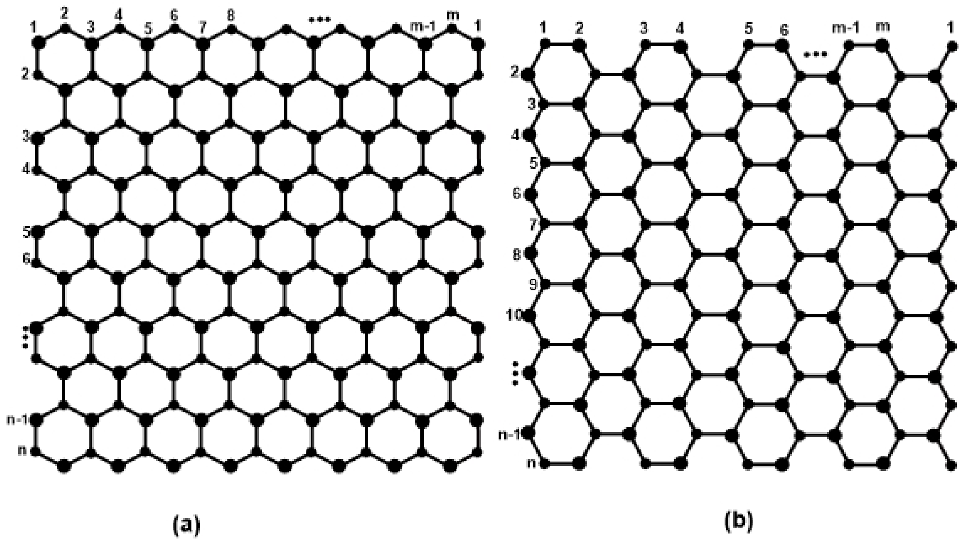


Figure 2. 2D models of: Zig-zag CNT (a); Armchair CNT (b).

Boron Triangular Nanotubes

A boron triangular nanotube, of order $n \times m$, is drawn from a hexagonal nanotube of the same order by adding a new vertex at the center of each hexagon and join it with the original points of the hexagon. Figure 3 shows the way of construction of a boron triangular nanotube.

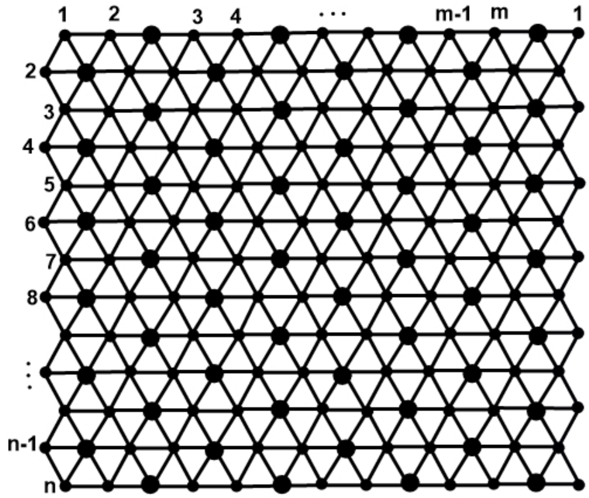


Figure 3. Boron triangular nanotube of order (n, m).

We denote the boron triangular nanotube of order $n \times m$ as $BNT_t[n, m]$, in which n is the number of rows and m is the number of columns. Since, there are $m(n-2)/2$ full hexagons and m half hexagons, the number of vertices is $3nm/2$ while that of edges is $3m(3n-2)/2$.

Figure 4. The dotted edges which need to be deleted from a full and a half hexagons.

Now we compute bipartite edge frustration of boron triangular nanotube.

Theorem 1. *Let $BNT_t[n, m]$ be the boron triangular nanotube with defining parameters n and m, then*

$$\phi(BNT_t[n, m]) = \frac{m}{2}(3n-2)$$

Proof. Consider *G* be a boron triangular nanotube. There exist no 2-coloring of *G* which results in $\phi(G) > 0$. To prove that it is exactly $\frac{m}{2}(3n-2)$, we need to prove both of the inequalities i.e. $\phi(G) \geq \frac{m}{2}(3n-2)$ and $\phi(G) \leq \frac{m}{2}(3n-2)$. Since a CNT has zero bipartite edge frustration, the problem is with the newly added edges. If one deletes three newly added alternating edges from a full hexagon and two newly added alternating edges from half hexagon that makes both full and half hexagons bipartite spanning subgraphs. Figure 4 exhibits the edges which need to be deleted from a full and a half hexagon. Since, there are $m(n-2)/2$ full hexagons and m half hexagons in a boron triangular nanotube, this implies that $\phi(G) \leq \frac{m}{2}(3n-2)$. On the other hand,one can easily be seen that there is no less number of edges to make the edges deleted subgraph a bipartite spanning subgraph. This turns out that $\phi(G) \geq \frac{m}{2}(3n-2)$ thus proving the theorem.

Boron α -Nanotubes

A boron α -nanotube of order $n \times m$ is obtained from a hexagonal nanotube of order $n \times m$ by deleting the central point of some hexagons of a triangular nanotube. We denote an (n,m)-boron α -nanotube as $BNT_{\alpha}[n,m]$ (Figure 5).

Lemma 2. *In an (n,m) -dimensional boron α -nanotube:*

- *There are $\frac{m}{2}(\frac{n}{3}-1)$ emptyl full hexagons.*
- *There are $\frac{m}{2}(\frac{2n}{3}-\frac{3}{2})$ filled full hexagons.*
- *There are $\frac{4nm}{3}$ vertices, when n is a multiple of 3.*
- *There are $\frac{m(7n-4)}{2}$ edges, when n is a multiple of 3.*

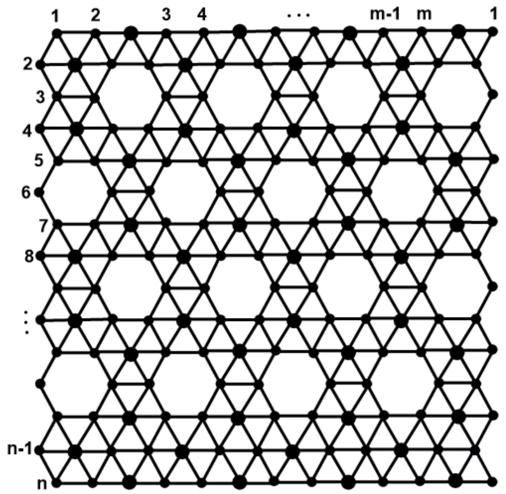


Figure 5. A 2D model of boron α -nanotube of order (n,m).

Let present the bipartite edge frustration of boron α-nanotube, $BNT_{\alpha}[n,m]$.

Theorem 3. Let $BNT_{\alpha}[n,m]$ be the (n,m)-dimensional boron α-nanotube, then

$$\phi(BNT_{\alpha}[n,m]) = \frac{m}{2}(2n+1)$$

Proof. Let *G* be the (n,m)-dimensional boron α-nanotube. Since we do not find any 2-coloring of G, it results that $\phi(G) > 0$. We prove both of the inequalities $\phi(G) \geq \frac{m}{2}(2n+1)$ and $\phi(G) \leq \frac{m}{2}(2n+1)$, to prove it is exactly $\frac{m}{2}(2n+1)$. If we delete three newly added alternative edges from a full hexagon and two newly added alternative edges from half hexagon it results in both full and half hexagons bipartite spanning subgraphs. Figure 4 exhibits the edges which need to be deleted from a full and a half hexagon. Since, there are $\frac{m}{2}(\frac{n}{3}-1)$ empty full hexagons and $\frac{m}{2}(\frac{2n}{3}-\frac{3}{2})$ filled hexagons in an (n,m)-dimensional boron α-nanotube, this implies that

$\phi(G) \leq \frac{m}{2}(2n+1)$. On the other hand, it can easily be seen that there is no less number of edges to make its edge deleted subgraph a bipartite spanning subgraph. This turns out that $\phi(G) \geq \frac{m}{2}(2n+1)$, which completes the proof.

CONCLUSIONS

Evaluating the bipartivity in chemical structures provides important information about their topology and eventually about chemical stability. Wile carbon polyhex nanotubes have zero bipartite edge frustration, the boron nanotubes have non-zero bipartivity.

ACKNOWLEDGMENTS

The first author is supported by CAS-TWAS president fellowship at USTC, China. The second author is partially supported by NUST, Pakistan.

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