

# On the SD- polynomial and SD- index of an infinite class of “Armchair Polyhex Nanotubes”

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## ABSTRACT

Let  $G$  be a simple connected graph with the vertex set  $V = V(G)$  and the edge set  $E = E(G)$ , without loops and multiple edges. For counting  $qoc$  strips in  $G$ , Diudea introduced the  $\Omega$ -polynomial of  $G$  and was defined as  $\Omega(G, x) = \sum_{i=1}^k x^{c_i}$ , where  $C_1, C_2, \dots, C_k$  be the “opposite edge strips” ops of  $G$  and  $c_i = |C_i|$  ( $i = 1, 2, \dots, k$ ). One can obtain the  $Sd$ -polynomial by replacing  $x^c$  with  $x^{|E(G)|-c}$  in  $\Omega$ -polynomial. Then the  $Sd$ -index will be the first derivative of  $Sd(x)$  evaluated at  $x = 1$ . In this paper we compute the  $Sd$ -polynomial and  $Sd$ -index of an infinite class of “Armchair Polyhex Nanotubes”.

**Keywords:** Omega and Sadhana polynomial; Sadhana index; Armchair Polyhex Nanotubes and Nanotori

## 1. INTRODUCTION

By a graph  $G$  means a pair  $G = (V, E)$  in which  $V = V(G)$  and  $E = E(G)$  denote to the set of vertices and edges, respectively. A chemical graph is a graph theoretical representation of a molecule whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. For two vertices  $x$  and  $y$  belong to  $V$ ,  $x$  is adjacent to  $y$  if and only if  $xy \in E(G)$ . In a connected graph, there is a path between every pair  $(x, y)$  of its vertices. The distance  $d(x, y)$  between vertices/atoms  $x$  and  $y$  ( $x, y \in V(G)$ ) is defined as the length of a shortest path between  $x$  and  $y$ . Two edges  $e = uv$  and  $f = xy$  of  $G$  are called co-distant, “ $e$  co  $f$ ”, if and only if they obey the following relation for a non-negative integer  $d$ : [1]

$$d(v, x) = d(v, y) + 1 = d(u, x) + 1 = d(u, y) = d$$

For some edges of  $G$  there are the following relations satisfied [1,2]:

$$e \text{ co } e$$

$$e \text{ co } f \Leftrightarrow f \text{ co } e$$

$$e \text{ co } f \ \& \ f \text{ co } h \Rightarrow e \text{ co } h$$

though the last relation is not always valid. In other words, the relation “co” is reflexive and symmetric but it is not necessary to be transitive. Set  $C(e) := \{f \in E(G), \mid e \text{ co } f\}$ , denote the subset of edges in  $G$ , co-distant to the edge  $e$ . If the relation “co” is transitive on  $C(e)$  then  $C(e)$  is called an *orthogonal cut* (denoted by *oc*) of  $G$ . The graph  $G$  is called *co-graph* if and only if the edge set  $E(G)$  a union of disjoint orthogonal cuts:  $E(G) = \cup_{i=1}^k C_i$  and  $C_i \cap C_j = \emptyset$ , for  $i \neq j$  and  $i, j = 1, 2, \dots, k$ .

If any two consecutive edges of an edge-cut sequence are topologically parallel within the same face of the covering, such a sequence is called a *quasi-orthogonal cut qoc* strip. For counting “opposite edge strips” qocs  $C_i$  of  $E(G)$  ( $i, j = 1, 2, \dots, k$ ), *M.V. Diudea* introduced the  $\Omega$ -polynomial of  $G$  [3-11] and was defined as  $\Omega(G, x) = \sum_{i=1}^k x^{c_i}$ , where  $c_i$ 's is the size of opposite edge strips ( $= |C_i|$  ( $i = 1, 2, \dots, k$ )).

It is easy to see that the first derivative of Omega polynomial  $\Omega(G, x)$  (in  $x = 1$ ) equals the number of edges in the graph

$$\Omega'(G, x) = \sum_{i=1}^k c_i = \sum_{i=1}^k |C_i| = |E(G)|$$

Another polynomial also related to the *ops* in  $G$  was introduced by *Ashrafi* and co-authors [12] in 2008, that counting the non-opposite edges is the *Sadhana* polynomial  $Sd(G, x)$  defined as:

$$Sd(G, x) = \sum_{i=1}^k x^{|E(G)|-c_i}$$

The *Sadhana* index  $Sd(G)$  for counting *qoc* strips in  $G$  was defined by *Khadikar et. al* [13,14] as first derivative of *sadhana* polynomial evaluated at  $x = 1$  [13-18]

$$Sd(G) = Sd'(G, x) = \sum_{i=1}^k (|E(G)| - c_i)$$

By definition of  $\Omega$ -polynomial, one can obtain the *Sd*-polynomial by replacing  $x^c$  with  $x^{|E(G)|-c}$  in  $\Omega$ -polynomial.

In chemical, physics and nano sciences, we have the appealing structure, especially symmetric structure with chemical constitution purporting. Carbon exists in several forms in nature. One is the so-called nanotube which was discovered for the first time in 1991 [19,20]. One of the nanotube is *Polyhex Nanotubes*, that the structure of polyhex nanotubes is consisting of the cycles with length six  $C_6$  in columns.

Since polyhex nanotubes have more practical in the chemical, physics and nano science, in this paper we focus on its structure and by using definition of *Sd*-polynomial and *Sd*-index, we compute these topological polynomial and index for an infinite class of Nano-structure “*Armchair Polyhex Nanotubes TUAC<sub>6</sub>*”, depicted in Figure 1.

Throughout this paper our notation is standard and mainly taken from standard book of graph theory such as [21-25].

## 2. RESULTS AND DISCUSSION

In this section we compute the  $Sd$ -polynomial and  $Sd$ -index of a family of *Polyhex Nanotubes*. In Figure 1, one can see that the 3-dimensional and 2-dimensional graph of Armchair polyhex nanotubes  $TUAC_6[m,n]$ , where  $m,n$  are the numbers of rows/columns of hexagon ( $C_6$ ) in 2-dimensional perception  $TUAC_6[m,n]$ . In a series of papers [26-36], some properties and applications and more historical details of nanotubes are presented and studied.

By these terminologies and from Figure 1, we will have the following results for *Armchair Polyhex Nanotubes*  $TUAC_6$ .

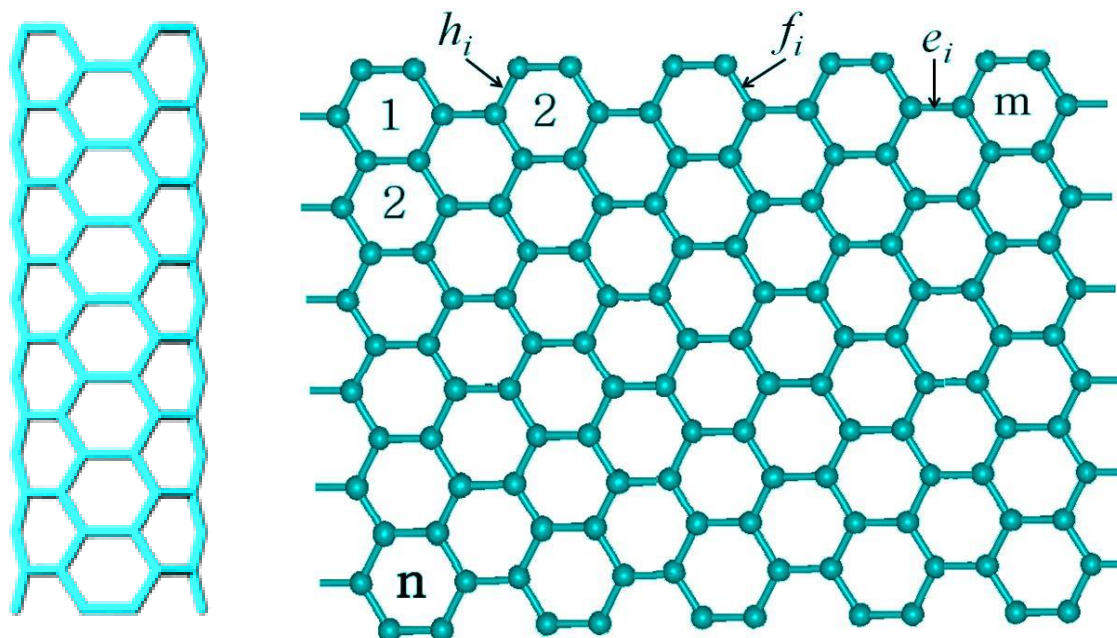
### Theorem 1.

$\forall m,n \in N$  let  $G = TUAC_6[m,n]$  be the Armchair polyhex nanotubes, then the  $Sd$ -polynomial and  $Sd$ -index of  $G$  are equal to

$$Sd(TUAC_6[m,n], x) = 2mx^{6mn+4m-n-1} + 2mx^{6mn+4m-2n-1}$$

and

$$Sd(TUAC_6[m,n]) = 24m^2n + 16m^2 - 6mn - 4m$$



**Fig. 1.** A 3-dimensional (left) and 2-dimensional (right) lattices of Armchair Polyhex Nanotubes  $TUAC_6[m,n]$ .

**Proof.**

Consider the Armchair polyhex nanotubes  $G = TUAC_6[m, n]$  ( $m, n \in \mathbb{N}$ ) (Figure 1). Let  $m, n$ ,  $|V(G)|$  and  $|E(G)|$  be the hexagons in rows/columns, number of vertices/carbon atoms and edges/chemical bonds of  $G$ . Then one can see that  $|V(G)| = 4m(n + 1)$  and  $|E(G)| = 6mn + 4m$ . Now, if we denote all horizontal edge in  $i^{\text{th}}$  column by  $e_i$  and all left (or right) oblique edges in  $i^{\text{th}}$  column by  $f_i$  (or  $h_i$ ), then it is easy to see that for all *quasi-orthogonal cuts*  $C_1, C_2, \dots, C_{2m}$ ,  $C_i = C(e_i)$  and also for all *quasi-orthogonal cuts*  $C_{2m+1}, C_{2m+2}, \dots, C_{3m}$ ,  $C_{2m+j} = C(f_j)$  and alternatively, for all *qocs*  $C_{3m+1}, C_{3m+2}, \dots, C_{4m}$ ,  $C_{3m+l} = C(h_l)$ .

Now by according to Figure 1, one can see that  $\forall i=1, 2, \dots, 2m: c_i = n + 1$  and  $\forall j = 1, 2, \dots, m: c_{2m+j} = c_{3m+j} = 2n + 1$ .

Thus, *Sd*-polynomial of Armchair polyhex nanotubes  $G = TUAC_6[m, n]$  is equal to

$$\begin{aligned} Sd(TUAC_6[m, n], x) &= \sum_{i=1}^k x^{|E(G)|-c_i} \\ &= 2m \times x^{6mn+4m-n-1} + m \times x^{6mn+4m-2n-1} + m \times x^{6mn+4m-2n-1} \end{aligned}$$

The *Sd*-polynomial of  $G$  implies that the *Sd*-index of  $TUAC_6[m, n]$  is equal to

$$\begin{aligned} Sd(TUAC_6[m, n]) &= Sd'(TUAC_6[m, n], x) = \left. \frac{\partial Sd(TUAC_6[m, n], x)}{\partial x} \right|_{x=1} \\ &= 2m \times (6mn + 4m - n - 1) + m \times (6mn + 4m - 2n - 1) + m \times (6mn \\ &\quad + 4m - 2n - 1) = 24m^2n + 16m^2 - 6mn - 4m \end{aligned}$$

Here, the proof is completed.

**3. CONCLUSION**

In this paper, we obtained the Sadhana polynomial and Sadhana index of Armchair Polyhex Nanotubes and Nanotori for the first time.

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