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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 *Ω-polynomial* of G and was defined as $\Omega(G, x) = \sum_{i=1}^{k} x^{c_i}$, where $C_1, C_2,..., C_k$ be the "opposite edge strips" ops of G and $c_i = |C_i|$ $(I = 1, 2,..., k)$. One can obtain the *Sd*-polynomial by replacing x^c with $x^{|E(G)|-c}$ in *Ω*-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 vrtices/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]:

$$e \ co \ e$$

$$e\ co\ f \Leftrightarrow f\ co\ e$$

$$e\ co\ f\ \&\ f\ co\ h \Rightarrow e\ co\ h$$

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 $C(e) := \{f \in E(G), \mid e\ co\ f\})$, denote the subset of edges in *G*, *c*o-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: $E(G) = \bigcup_{i=1}^{k} C_i$ and $C_i \cap C_j = \emptyset$, for $i \neq j$ and $i,j = 1, 2, \ldots, k$.

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 $E(G)$ $(i, j = 1, 2, \ldots, k)$, *M.V. Diudea* introduced the *Ω-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 $(= |C_i|\ (i = 1, 2, \ldots, k))$.

It is easy to see that the first derivative of Omega polynomial *Ω(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]

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

By definition of *Ω*-polynomial, one can obtain the *Sd*-polynomial by replacing x^c with $x^{|E(G)|-c}$ in *Ω*-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* $TUAC_6$", depicted in Figure 1.

Throghout 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-dimentional and 2-dimentional graph of Armchair polyhex nanotubes $TUAC_6[m,n]$, where m,n are the numbers of rows/columns of hexagon (C_6) in 2-dimentional 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 studed.

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 equale to

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

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

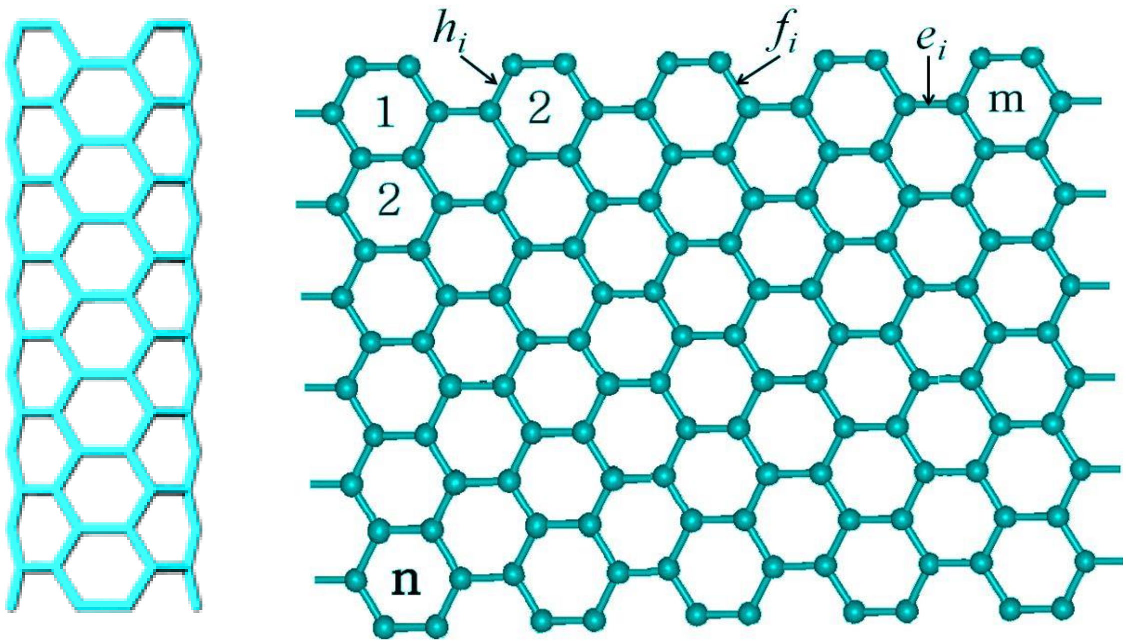

Fig. 1. A 3-dimentional (left) and 2-dimentional (right) lattices of Armchair Polyhex Nanotubes $TUAC_6[m,n]$.

Proof.

Consider the Armchair polyhex nanotubes $G = TUAC_6[m,n]$ $(m,n \in N)$ (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 hotizontal edge in i^{th} column by e_i and all left (or right) oblique edges in i^{th} column by f_i (or h_i), then it is easy to see that for all *quasi-orthogonal cuts* $C_1, C_2,..., C_{2m}$, $C_i = C(e_i)$ and also for all *quasi-orthogonal cuts* $C_{2m+1}, C_{2m+2},..., C_{3m}$, $C_{2m+j} = C(f_j)$ and alternatively, for all *qocs* $C_{3m+1}, C_{3m+2},..., C_{4m}$, $C_{3m+l} = C(h_l)$.

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

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

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

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

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

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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