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Vertex PI_v Topological Index of Titania Carbon Nanotubes $TiO_2(m,n)$

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Abstract

A topological index of a graph G is a numeric quantity related to G which is invariant under automorphisms of G. The Padmakar-Ivan (PI) index of a graph G is defined as $PI(G) = \sum_{e=uv\in E(G)} [n_u + n_v]$, where n_u is the number of edges of G lying closer to v than u, analogously n_v. In this paper, we compute the vertex PI index of *Titania carbon Nanotubes* $TiO_2[m,n]$.

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1 Introduction

Let G be a connected graph with vertex and edge sets $V(G)$ and $E(G)$, respectively. As usual, the distance between the vertices u and v of G is the number of edges in a minimal path connecting them, denoted as $d(u,v)$. Define $N_G(u)$ to be the set of all vertices adjacent to u. The *diameter* is the greatest distance between two vertices of G, denoted as $diam(G)$.

Let $e=uv$ be an edge of the graph G. The number of vertices of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $n_u(e)$. Analogously, $n_v(e)$ is the number of vertices of G whose

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distance to the vertex v is smaller than the distance to the vertex u.

Suppose X denoted the class of all graphs. A map *Top* from X into real numbers is called a topological index if $G \cong H$implies that $Top(G) = Top(H)$. Obviously, the maps $Top_v$and Top_e defined as the number of edges and vertices respectively, are topological indices.

The *Wiener index* was the first reported topological index based on graph distances [1]. This index is defined as the sum of all distances between vertices of the graph under consideration. The *Wiener index* is applicable to acyclic graphs only. For cyclic compounds a novel molecular graph based descriptor, referred to as the *Szeged index* [2]. This is considered as the modification of Wiener index to cyclic graph. The Szeged index is defined as

$$Sz(G) = \sum_{e=uv\in E(G)} n_u \cdot n_v$$

Note that vertices equidistant to u and v are not counted.

For acyclic graphs the Szeged and Wiener indices coincide. As a consequence, *Padmaker* and *Ivan* introduced another index called *Padmakar-Ivan index* (PI_v) [3,4]. PI of a graph G is defined as

$$PI_v(G) = \sum_{e=uv\in E(G)} (n_u + n_v).$$

Note that vertices equidistant to u and v are not counted. Many methods for the calculation of these indices of some systems are considered in [5–11].

As a well-known semiconductor with numerous technological applications, Titania nanotubes are comprehensively studied in material sciences. Titania nanotubes were systematically synthesized during the last 10-15 years using different methods and carefully studied as prospective technological materials. Since the growth mechanism for TiO_2nanotubes is still not well defined, their comprehensive theoretical studies attract enhanced attention. The TiO_2 sheets with a thickness of a few atomic layers were found to be remarkably stable.

In this paper, we compute the vertex PI index of the Titania nanotubes. For further results we refer [12–14].

2 Main Results

The 2-dimensional graph of the Titania nanotube, $TiO_2[m,n]$, is shown in Figure 1, where m and n denotes the number of octagons in a column and the number of octagons in a row of the Titania nanotube. This graph has $2(3n+2)(m+1)$ vertices and $10mn + 6m + 8n + 4$ edges.

By using the *orthogonal cuts* and *cut method* of the Titania nanotubes, we can determine all edge cuts of the Titania nanotubes. The edge cut $C(e)$ is an orthogonal cut, such that the set of all edges $f \in E(G)$ are strongly co-distant to e. For further research and study of the cut method and orthogonal cuts in some classes of chemical graphs see [8,9,11,15].

By using the cut method and finding orthogonal cuts, we can compute the quantities of $n_u(e|TiO_2[m,n])$ and $n_v(e|TiO_2[m,n])$, $\forall e \in E(TiO_2[m,n])$, which are the number of vertices in two sub-graphs $TiO_2[m,n]$-$C(e)$. In case the Titania Nanotubes $TiO_2[m,n]$ $\forall e=uv \in E(TiO_2[m,n])$, we denote $n_u(e|TiO_2[m,n])$ as the number of vertices in the left component of $TiO_2[m,n]$-$C(e)$ and alternatively $n_v(e|TiO_2[m,n])$ as the number of vertices in the right component of $TiO_2[m,n]$-$C(e)$, since all edges in $TiO_2[m,n]$ Nanotubes sheets are oblique or horizontal.

Theorem 1. *Let* $TiO_2[m,n]$ *be the Titania Nanotubes, where* $m,n \in N$. *Then vertex PI index of* $TiO_2[m,n]$ *is:*

$$PI_v(TiO_2(m,n)) = 2(m+1)(3n+2)(n+1)(11m+9)$$

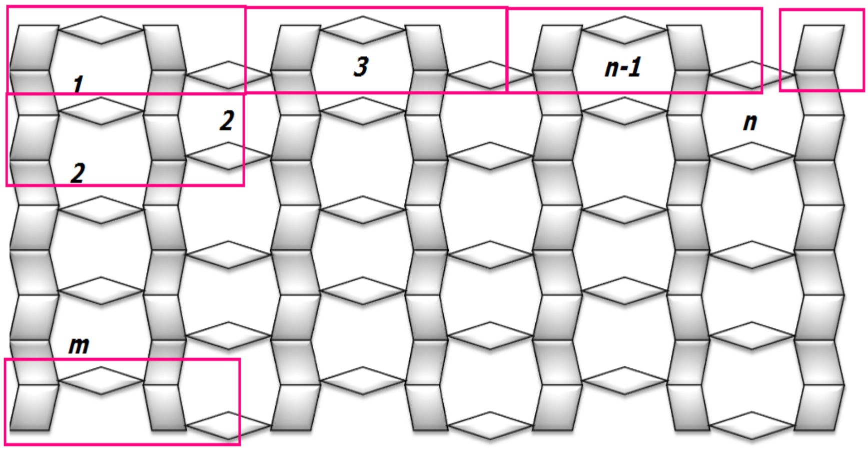

Fig. 1 2-dimensional model to Titania nanotube $TiO_2[m,n]$.

Proof. According to the structure of the Titania Nanotubes $TiO_2[m,n]$ for all integer numbers $m,n>1$, we have following results:

For the edge $e_1=u_1v_1$ that belong to the first square of $TiO_2[m,n]$ Nanotubes (in the first column and row), we see that

$$n_{u1}(e_1|TiO_2[m,n])=2(m+1)$$

$$n_{v1}(e_2|TiO_2[m,n])=6mn+4m+6n+4-2(m+1)=6mn+2m+6n+2.$$

For the edge $e_2=u_2v_2$:

$$n_{u2}(e_2|TiO_2[m,n])=3\times 2(m+1)+1\times 2(m+1)=8(m+1)$$

and

$$n_{v2}(e_2|TiO_2[m,n])=6mn+4m+6n+4-8(m+1)=6mn-4m+6n-4.$$

For the edge $e_{n+1}=u_{n+1}v_{n+1}$:

$$n_{un+1}(e_{n+1}|TiO_2[m,n])=(3n+1)\times 2(m+1)$$

and

$$n_{vn+1}\ (e_{n+1}|TiO_2[m,n])=6mn+4m+6n+4-(6mn+6n+2m+2)=2(m+1).$$

Thus, by a simple induction for $i=1,2,\ldots,n;$ we can see that for the edge $e_i=u_iv_i$:

$$n_{ui}(e_i|TiO_2[m,n])=2(m+1)\times(3(i-1)+1)$$

and

$$\begin{aligned} n_{vi}(e_i|TiO_2[m,n])&=6mn+4m+6n+4-(6mi+6i-4m-4)\\ &=6m(n-i)+6(n-i)+8(m+1)\\ &=6(m+1)(n-i)+8(m+1)\\ &=2(m+1)(3(n-i)+4). \end{aligned}$$

Let the edge $f_1=u_1v_1\in E(TiO_2[m,n])$ be the first oblique edge in the first square of $TiO_2[m,n]$ Nanotubes (in the first column and row), we see that

$$n_{u1}(f_1|TiO_2[m,n])=m+1$$

and

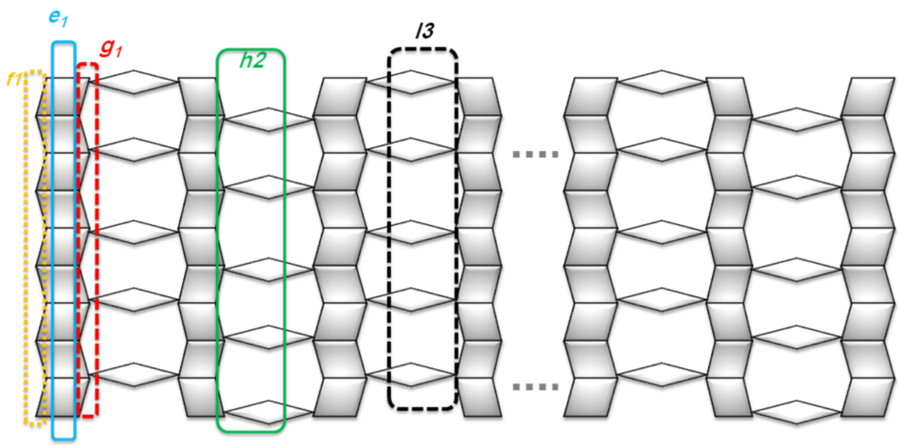

Fig. 2 Categories for edges of the Titania Carbon Nanotubes.

$$\begin{aligned} n_{v1}(f_1|TiO_2[m,n]) &= 6mn+4m+6n+4-(m+1) \\ &= 6mn+3m+6n+3 \\ &= 6n(m+1)+3(m+1) \\ &= (6n+3)(m+1). \end{aligned}$$

For the edge $f_2=u_2v_2$:

$$n_{u2}(f_2|TiO_2[m,n])=(m+1)+3\times 2(m+1)=7(m+1)$$

and

$$n_{v2}(f_2|TiO_2[m,n])=6mn+4m+6n+4-7(m+1)=6n(m+1)-3(m+1)=(6n-3)(m+1).$$

For the edge $f_{(n+1)}=uv$:

$$n_{u(n+1)}(f_{(n+1)}|TiO_2[m,n])=(m+1)+3n\times 2(m+1)=(6n+1)(m+1)$$

and

$$n_{v(n+1)}(f_{(n+1)}|TiO_2[m,n])=(6n+4)(m+1)-(6n+1)(m+1)=3(m+1).$$

Therefore, by a simple induction for $j=1,2,\ldots,n+1;$ we can proof the previous statement.

For the edge $f_j=u_jv_j$:

$$n_{uj}(f_j|TjO_2(m,n))=3(j-1)\times 2(m+1)+(m+1)=(m+1)(6j-5)$$

and

$$\begin{aligned} n_{vj}(f_j|TjO_2(m,n)) &= (6n+4)(m+1)-(m+1)(6j-5) \\ &= (m+1)(6n-6j+9) \\ &= 3(m+1)(2n+3-2j). \end{aligned}$$

Let the edge $g_1=u_1v_1\in E(TiO_2[m,n])$ be the second oblique edge in the first square of $TiO_2[m,n]$ Nanotubes (in the first column and row), so we have

$$n_{u1}(g_1|TiO_2[m,n])=2(m+1)+(m+1)$$

and

$$n_{v1}(g_1|TiO_2[m,n])=(6n+4)(m+1)-3(m+1)=(6n+1)(m+1)$$

For $g_2=u_2v_2$:

$$n_{u2}(g_2|TiO_2[m,n])=3\times 2(m+1)+2(m+1)+(m+1)=9(m+1)$$

and

$$n_{v2}(g_2|TiO_2[m,n])=(6n+4)(m+1)-9(m+1)=(6n-5)(m+1)$$

For $g_{n+1}=u_{n+1}v_{n+1}$:

$$n_{un+1}(g_{n+1}|TiO_2[m,n])=3n\times 2(m+1)+2(m+1)+(m+1)=(6n+3)(m+1)$$

and

$$n_{vn+1}(g_{n+1}|TiO_2[m,n])=(6n+4)(m+1)-(6n+3)(m+1)=(m+1).$$

And these imply that $\forall j=1,2,\ldots,n+1$

$$n_{uj}(g_j|TjO_2(m,n))=3j\times 2(m+1)+3(m+1)=(m+1)(6j+3)$$

and

$$n_{vj}(g_j|TjO_2(m,n))=(6n+4)(m+1)-(m+1)(6j+3)=(m+1)(6n-6j+1).$$

Finally, let $h_1=u_1v_1$ & $l_2=u_2v_2\in E(TiO_2[m,n])$ be the first and second oblique edges in the second square of the first row (or the first square in the second column) of $TiO_2[m,n]$ Nanotubes, then

$$n_{u1}(h_1|TiO_2[m,n])=2\times 2(m+1)$$

and

$$n_{u2}(l_2|TiO_2[m,n])=3\times 2(m+1)$$

$$n_{v1}(h_1|TiO_2[m,n])=(6n+4)(m+1)-2(m+1)=(6n+2)(m+1)$$

and

$$n_{v2}(l_2|TiO_2[m,n])=(6n+1)(m+1)$$

And by a simple induction on $\forall i=1,2,\ldots,n;$ for the edges $h_i=u_iv_i$and $l_i=a_ib_i$ we have

$$n_{ui}(h_i|TiO_2[m,n])=3(i-1)\times 2(m+1)+2\times 2(m+1)=2(m+1)(3i-1)$$

and

$$\begin{aligned} n_{vi}\,(h_i|TiO_2[m,n]) &=(6n+4)(m+1)-2(m+1)(3i-1)\\ &=(m+1)(6n-6i+6)\\ &=6(m+1)(n+1-i).\end{aligned}$$

$$n_{ai}(l_i|TiO_2[m,n])=3(i-1)\times 2(m+1)+3\times 2(m+1)=6i(m+1)$$

and

$$\begin{aligned} n_{bi}\,(l_i|TiO_2[m,n]) &=(6n+4)(m+1)-6i(m+1)\\ &=(m+1)(6n-6i+4)\\ &=3(m+1)(3n+2-2i).\end{aligned}$$

On the other hands, by according to Figure 2, we can see that the size of all orthogonal cuts for these edge categories in the Titania Nanotubes $TiO_2[m,n]$ are equal to ($\forall i=1,2,\ldots,n+1$):

$$|C(e_i)|=|C(h_i)|=|C(l_i)|=2(m+1)$$

and

$$|C(f_i)|=|C(g_i)|=2m+1.$$

From the above calculations and Figure 2, we can compute the vertex PI index of Titania Nanotubes $TiO_2[m,n]$.

$$PI_v(TiO_2[m,n])=\sum_{e=uv\in E(G)}\left(n_u(e|TiO_2(m,n)+n_v(e|TiO_2(m,n))\right)$$

$$=\sum_{\substack{e_i=uv\in E(TiO_2(m,n))\\ \forall i=1,2,\ldots,n+1}}|C(e_i)|\left(n_u(e_i|TiO_2(m,n))+n_v(e_i|TiO_2(m,n))\right)$$

$$+ \sum_{\substack{f_i = uv \in E(TiO_2(m,n)) \\ \forall i = 1,2,\ldots,n+1}} |C(f_i)| \left[n_u(f_i|TiO_2(m,n)) + n_v(f_i|TiO_2(m,n)) \right]$$

$$+ \sum_{\substack{g_i = uv \in E(TiO_2(m,n)) \\ \forall i = 1,2,\ldots,n+1}} |C(g_i)| \left[n_u(g_i|TiO_2(m,n)) + n_v(g_i|TiO_2(m,n)) \right]$$

$$+ \sum_{\substack{h_i = uv \in E(TiO_2(m,n)) \\ \forall i = 1,2,\ldots,n}} |C(h_i)| \left[n_u(h_i|TiO_2(m,n)) + n_v(h_i|TiO_2(m,n)) \right]$$

$$+ \sum_{\substack{l_i = uv \in E(TiO_2(m,n)) \\ \forall i = 1,2,\ldots,n}} |C(l_i)| \left[n_u(l_i|TiO_2(m,n)) + n_v(l_i|TiO_2(m,n)) \right]$$

$$\begin{aligned} &= \textstyle\sum_{i=1}^{n+1} 2(m+1)\left(2(m+1)(3(i-1)+1) + 2(m+1)(3(n-i)+4)\right) \\ &+ \textstyle\sum_{i=1}^{n+1} 2(m+1)\left((m+1)(6i-5) + 3(m+1)(2n+3-2i)\right) \\ &+ \textstyle\sum_{i=1}^{n+1} 2(m+1)\left((m+1)(6i+3) + (m+1)(6n-6i+1)\right) \\ &+ \textstyle\sum_{i=1}^{n} (2m+1)\left(2(m+1)(3i-1) + (m+1)(n+1-i)\right) \\ &+ \textstyle\sum_{i=1}^{n} (2m+1)\left(6i(m+1) + 3(m+1)(3n+2-2i)\right) \end{aligned}$$

$$= 4(m+1)^2 \sum_{i=1}^{n+1}(3n+2) + (2m+1)(m+1)\sum_{i=1}^{n+1}(6n+4) + (2m+1)(m+1)\sum_{i=1}^{n+1}(6n+4) +$$

$$4(m+1)^2 \sum_{i=1}^{n+1}(3n+2) + 6(m+1)^2 \sum_{i=1}^{n+1}(3n+2)$$

$$= 4(m+1)^2(3n+2)(n+1) + (2m+1)(m+1)(6n+4)(n+1) + (2m+1)(m+1)(6n+4)(n+1)$$

$$+4(m+1)^2(3n+2)(n+1) + 6(m+1)^2(3n+2)(n+1)$$

$$= 2(m+1)(3n+2)(n+1)(11m+9)$$

which is the required result and the proof is over

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