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Research Article

Edge-Vertex Szeged Index of Titania Nanotube $TiO_2(m,n), \forall m,n \geq 1$

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ABSTRACT:
For a connected graph G, the vertex-Szeged and the edge-Szeged index is defined as $Sz_v(G)=\sum_{e=uv}\left[n_u(e|G)\times n_v(e|G)\right]$ and $Sz_e(G)=\sum_{e=uv}\left[m_u(e|G)\times m_v(e|G)\right]$, respectively, where $n_u(e|G)$ is the number of vertices of G lying closer to u than v and $m_u(e|G)$ is the number of edges lying closer to the vertex u then the vertex v in G. Recently, the edge-vertex Szeged index is introduced which is defined as $Sz_{ev}=\frac{1}{2}\sum_{e=uv\in E(G)}\left[n_u(e|G)\times m_v(e|G)+m_u(e|G)\times n_v(e|G)\right]$.

In this paper, we compute the exact formula of edge-vertex Szeged index for the Titanai nanotube $TiO_2(m;n)$ graph.

Keywords: *Edge-vertex Szeged index, orthogonal cuts, Titania nanoutbe TiO2(m;n).*

[I] NTRODUCTION

Titania nanotube TiO_2 is one of the most studied compounds in materials science. Some outstanding properties it is used for in photocatalysis, biomedical and dye-sensitized solar cells. In 1999, rst reports showed the feasibility to grow highly ordered arrays of TiO_2 nanotubes by a simple but optimized electrochemical anodization of a titanium meta sheet. This finding stimulated intense research activities that focused on growth, modification, properties and applications of these one-dimensional nanostructures [13].

Let G be a connected graph with the vertex set V(G) and the edge set E(G). The distance, $d_G(u;v)$, between two vertices $u;v \in V(G)$ in a graph G is the length of the shortest path between them. For an edge $e=uv \in E(G)$, $n_u(e|G)$ is the number of vertices of G lying closer to u than to v, analogously $n_v(e|G)$, $m_u(e|G)$ is the number of edges of G lying closer to u than to v, analogously defined $m_v(e|G)$, and $t_u(e|G)$ is the number of vertices and edges of G whose distance to vertex u is smaller than the distance to vertex v, and $t_v(e|G)$ defined analogously i.e.

The Wiener index is one of the oldest and the most thoroughly studied topological indices. The Wiener index of a graph G is defined as [3, 11, 27]

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)$$

In 1995, I. Gutman [6] introduced another distance based topological index named as Szeged index (vertex Szeged index).

$$Sz_v(G) = \sum_{e=uv} \left[n_u(e|G) \times n_v(e|G) \right]$$

The edge version of Szeged index introduced by A. R. Ashrafi [4] and it is defined as

$$Sz_e(G) = \sum_{e=uv} \left[m_u(e|G) \times m_v(e|G) \right],$$

The edge-vertex-Szeged index [4] of the graph G is defined as

$$Sz_{ev} = \frac{1}{2} \sum_{e=uv \in E(G)} \left[n_u(e|G) \times m_v(e|G) + m_u(e|G) \times n_v(e|G) \right]$$

and the total-Szeged index is defined as

$$Sz_T(G) = \sum_{e \in E(G)} t_u(e|G) \times t_v(e|G)$$

or

$Sz_T(G) = Sz_v(G) + Sz_e(G) + 2Sz_{ev}(G)$

For further details and results on Szeged indices we refer [2, 5, 7, 10, 12,14]

S. Klavžar gave the general description of the cut method and Johan et. al describes orthogonal cut by using the term of strongly co-distant. For detail study on cut vertex see [8, 9].

[II] MATERIALS AND METHODS

In this section, we computed the edge-vertex Szeged and the total Szeged indices of titania nanotube $TiO_2(m;n)$. The two dimensional lattice of titania nanotube $TiO_2(m;n)$ is shown in Figure 1, where m and n represent the number of octagons in a column and in a row, respectively, of the titania nanotube. The general representation of $TiO_2(m;n)$ have *2(3n+2)(m+1)* vertices and *10mn+6m+8n+4* edges [15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26].

Theorem 1. Let the graph of Titania nanotube $TiO_2(m;n)$, for all m;n>1, then the edge-vertex Szeged index of $TiO_2(m;n)$ is equal to:

$$Sz_{ev} = \frac{1}{2}\big[15 + 93n + 246n^2 + 136n^3 + 12mn(8 + 74n + 45n^2)$$
$$+ m^2(90 + 232n - 198n^2 - 208n^3) + 2m^3(20 + 85n + 192n^2 + 105n^3)$$
$$+ m(65 + 251n - 24n^2 - 66n^3 + 12mn(16 + 100n + 63n^2))\big]$$

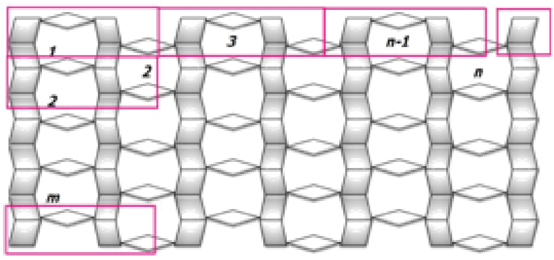

Figure 1: 2-dimensional representation of Titania Nanotutbe $TiO_2(m;n)$.

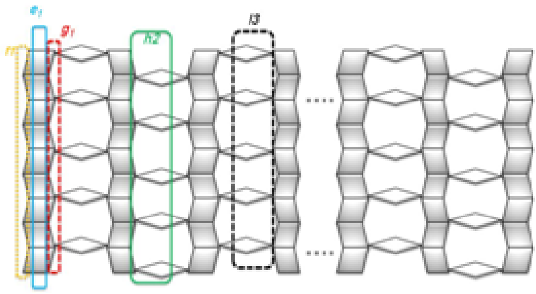

Figure 2: Edge partition of the Titania Carbon Nanotubes $TiO_2(m,n)$.

Proof. To obtain the final result, we partitioned the vertex and the edge sets with the help of cut method and orthogonal cuts of the TiO_2, Fig. 2. With the help of this partition we computed the quantities $n_u(e|TiO_2(m;n))$ *and* $n_v(e|TiO_2(m;n))$; $\forall e \in E(TiO2(m,n))$, which are the number of vertices in two sub-graphs $TiO_2(m;n)$-$C(e)$, where $C(e) = \{f \in E(TiO_2(m,n))\} \mid f \text{ is co-distant with } e\}$. So $\forall m,n > 1$, we have the following information.

For $e_1 = u_1 v_1$

$n_{u_1}(e_1 \mid TiO_2(m,n)) = 2(m+1)$

$n_{v_1}(e_1 \mid TiO_2(m,n)) = 6mn + 4m + 6n$
$+4 - 2(m+1) = 6mn + 2m + 6n + 2.$

For $e_2 = u_2 v_2$

$n_{u_2}(e_2 \mid TiO_2(m,n))$
$= 3 \times 2(m+1) + 1 \times 2(m+1) = 8(m+1)$

$n_{v_2}(e_2 \mid TiO_2(m,n)) = 6mn + 4m + 6n$
$+4 - 8(m+1) = 6mn - 4m + 6n - 4.$

For $e_{n+1} = u_{n+1} v_{n+1}$

$n_{u_{n+1}}(e_{n+1} \mid TiO_2(m,n)) = (3n+1) \times 2(m+1)$

$n_{v_{n+1}}(e_{n+1} \mid TiO_2(m,n)) = 6mn + 4m + 6n$
$+4 - (6mn + 6n + 2m + 2) = 2(m+1).$

Thus, by induction we noticed that for edges $e_i = u_i v_i, i = 1, 2, \cdots, n$:

$n_{u_i}(e_i \mid TiO_2(m,n)) = 2(m+1) \times (3(i-1)+1)$

$n_{v_i}(e_i \mid TiO_2(m,n)) = 6mn + 4m + 6n + 4$
$-(6mi + 6i - 4m - 4) = 2(m+1)(3(n-i)+4)$

For $f_1 = u_1 v_1$

$n_{u_1}(f_1 \mid TiO_2(m,n)) = m+1$

$n_{v_1}(f_1 \mid TiO_2(m,n)) = 6mn + 4m + 6n$
$+4 - (m+1) = (6n+3)(m+1)$

For $f_1 = u_1 v_1$

$n_{u_2}(f_2 \mid TiO_2(m,n))$
$= (m+1) + 3 \times 2(m+1) = 7(m+1)$

$n_{v_2}(f_2 \mid TiO_2(m,n)) = 6mn + 4m + 6n$
$+4 - 7(m+1) = (6n-3)(m+1).$

For $f_{n+1} = u_{n+1} v_{n+1}$

$n_{u_{(n+1)}}(f_{n+1} \mid TiO_2(m,n))$
$= (m+1) + 3n \times 2(m+1) = (6n+1)(m+1)$

$n_{v_{n+1}}(f_{n+1} \mid TiO_2(m,n))$
$= (6n+4)(m+1) - (6n+1)(m+1) = 3(m+1).$

Thus, by induction we noticed that for edges $f_i = u_i v_i, i = 1, 2, \cdots, n+1$:

For $f_i = u_i v_i$

$n_{u_i}(f_i \mid TiO_2(m,n)) = 3(i-1) \times 2(m+1)$
$+(m+1) = (m+1)(6i-5)$

$n_{v_i}(f_i \mid TiO_2(m,n)) = (6n+4)(m+1)$
$-(m+1)(6i-5) = 3(m+1)(2n-2i+3)$

For $g_1 = u_1 v_1$

$n_{u_1}(g_1 \mid TiO_2(m,n)) = 2(m+1) + (m+1)$

$n_{v_1}(g_1 \mid TiO_2(m,n)) = (6n+4)(m+1)$
$-3(m+1) = (6n+1)(m+1)$

For $g_2 = u_2 v_2$

$n_{u_2}(g_2 \mid TiO_2(m,n)) = 3 \times 2(m+1)$
$+2(m+1) + (m+1) = 9(m+1)$

$n_{v_2}(g_2 \mid TiO_2(m,n)) = (6n+4)(m+1)$
$-9(m+1) = (6n-5)(m+1)$

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

$n_{u_{n+1}}(g_{n+1} \mid TiO_2(m,n)) = 3n \times 2(m+1)$
$+2(m+1) + (m+1) = (6n+3)(m+1)$

$n_{v_{n+1}}(g_{n+1} \mid TiO_2(m,n)) = (6n+4)(m+1)$
$-(6n+3)(m+1) = (m+1).$

Thus, by induction we noticed that for edges $g_i = u_i v_i, i = 1, 2, \cdots, n+1$

For $g_i = u_i v_i$

$n_{u_i}(g_i \mid TiO_2(m,n)) = 3i \times 2(m+1)$
$+3(m+1) = (m+1)(6i+3)$

$n_{v_i}(g_i \mid TiO_2(m,n)) = (6n+4)(m+1)$
$-(m+1)(6i+3) = (m+1)(6n-6i+1)$

For $h_1 = u_1 v_1$

$n_{u_1}(h_1 \mid TiO_2(m,n)) = 2 \times 2(m+1)$

$n_{v_1}(h_1 \mid TiO_2(m,n)) = (6n+4)(m+1)$

$-2(m+1) = (6n+2)(m+1)$

By induction we noticed that for edges $g_i = u_i v_i, i = 1, 2, \cdots, n+1,$

For $h_i = u_i v_i$

$n_{u_i}(h_i \mid TiO_2(m,n)) = 3(i-1) \times 2(m+1)$

$+2 \times 2(m+1) = 2(m+1)(3i-1)$

$n_{v_i}(h_i \mid TiO_2(m,n)) = (6n+4)(m+1)$

$-2(m+1)(3i-1)$

For $l_1 = u_1 v_1$

$n_{u_1}(l_1 \mid TiO_2(m,n)) = 3 \times 2(m+1)$

$n_{v_1}(l_1 \mid TiO_2(m,n)) = (6n+1)(m+1)$

By induction we noticed that for edges $g_i = u_i v_i, i = 1, 2, \cdots, n+1,$

For $l_i = u_i v_i$

$n_{a_i}(l_i \mid TiO_2(m,n)) = 3(i-1) \times 2(m+1)$

$+3 \times 2(m+1) = 6i(m+1)$

$n_{b_i}(l_i \mid TiO_2(m,n)) = (6n+4)(m+1)$

$-6i(m+1) = 3(m+1)(3n+2-2i).$

We also observed the following

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

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

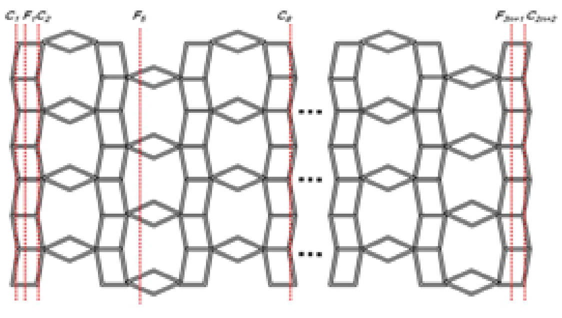

Figure 3: Orthogonal cuts representation of the Titania nanotubes.

From Fig. 3, we notice that there are 5n+3 vertical cuts for all edges in the graph of TiO_2(m;n) and clearly all these cuts are vertical. Every edge e in the graph of TiO_2(m;n) is either an oblique or a horizontal edge. We denote orthogonal cuts by C_i (for oblique edges) and F_j (for horizontal edges), where $i = 1, \cdots, 2(n+1)$ and $j = 1, \cdots, 3n+1$. Also, notice that $|C_i|$=2m+1 and $|F_j|$=2(m+1) for all orthogonal cuts. Now we compute the terms m_u and m_v for each edge uv of the graph TiO_2(m;n).

For $C_{(2h-1)}$:

$m_u(e_{(2h-1)} \mid TiO_2(m,n)) = (10m+8)(h-1)$

$m_v(e_{(2h-1)} \mid TiO_2(m,n)) = 10mn + 6m + 8n$

$+4 - (10m+8)(h-1) - (2m+1)$

For C_{2h}:

$m_u(e_{(2h)} \mid TiO_2(m,n)) = 10hm + 8h - 6m - 5,$

$m_v(e_{(2h)} \mid TiO_2(m,n)) = 10m(n-h) + 10m + 8(n-h) + 8.$

For $F_{3h+1}(h = 0, \ldots, n)$

$m_u(F_{3h+1} \mid TiO_2(m,n)) = 10hm + 2m + 8h + 1,$

$m_v(F_{3h+1} \mid TiO_2(m,n)) = (10m+8)(n-h) + 4m + 3.$

For $F_{3h-1}(h = 1, \ldots, n)$:

$m_u(F_{3h-1} \mid TiO_2(m,n)) = 10hm - 4m + 8h - 4,$

$mv(F_{3h-1} \mid TiO_2(m,n)) = (10mn + 6m + 8n + 4)$

$-(10hm - 4m + 8h - 4) = (10m+8)(n-h) + 10m + 8.$

For $F_{3h}(h = 1, \ldots, n)$:

$m_u(F_{3h} \mid TiO_2(m,n)) = (10m+8)h - 2m - 2,$

$m_v(F_{3h} \mid TiO_2(m,n)) = m_v(F_{3h-1} \mid TiO_2(m,n))$

$-|F1| = (10m+8)(n-h) + 8m + 6.$

From the above calculations and observations, now we are able to find the edge-vertex Szeged index of the graph of the Titania nanotube TiO_2.

$$Sz_{ev}(TiO_2(m,n)) = \frac{1}{2}\sum_{e \in E(TiO_2(m,n))}\left[n_u(e \mid TiO_2(m,n)) \times m_v(e \mid TiO_2(m,n)) + n_v(e \mid TiO_2(m,n)) \times m_u(e \mid TiO_2(m,n))\right]$$

$$= \frac{|C_1|}{2}\sum_{\substack{e_{2h-1}=vu \in C_{2h-1} \\ h=1,\ldots,n+1}}\left[m_u\left(e_{2h-1} \mid TiO_2(m,n)\right) \times 2(m+1)\left(3(n-h)+4\right) + 2(m+1)\left(3(h-1)+1\right) \times m_v\left(e_{2h-1} \mid TiO_2(m,n)\right)\right]$$

$$+\frac{|C_1|}{2}\sum_{\substack{e_{2h}=vu\in C_{2h}\\ h=1,\ldots,n+1}}\left[m_u\left(e_{2h}\mid TiO_2(m,n)\right)\times 3(m+1)(2n+3-2h)+(m+1)(6h-5)\times m_v\left(e_{2h}\mid TiO_2(m,n)\right)\right]$$

$$+\frac{|F_1|}{2}\sum_{\substack{f_{3k+1}=vu\in F_{3k+1}\\ k=1,\ldots,n}}\left[m_u\left(f_{3k+1}\mid TiO_2(m,n)\right)\times(m+1)(6n-6k+1)+(m+1)(6k+3)\times m_v\left(f_{3k+1}\mid TiO_2(m,n)\right)\right]$$

$$+\frac{|F_1|}{2}\sum_{\substack{f_{3k}=vu\in F_{3k}\\ k=1,\ldots,n}}\left[m_u\left(f_{3k}\mid TiO_2(m,n)\right)\times(m+1)(n+1-k)+(m+1)(6k+3)\times m_v\left(f_{3k}\mid TiO_2(m,n)\right)\right]$$

$$+\frac{|F_1|}{2}\sum_{\substack{f_{3k-1}=vu\in F_{3k-1}\\ k=1,\ldots,n}}\left[m_u\left(f_{3k-1}\mid TiO_2(m,n)\right)\times 3(m+1)(3n+2-2k)+6k(m+1)\times m_v\left(f_{3k-1}\mid TiO_2(m,n)\right)\right]$$

$$=\frac{|C_1|}{2}\sum_{\substack{e_{2h-1}=vu\in C_{2h-1}\\ h=1,\ldots,n+1}}\left[(10m+8)(h-1)\times(2(m+1)(3(n-h)+4))\right.$$

$$\left.+(10mn+6m+8n+4-(10m+8)(h-1)-(2m+1))\times(2(m+1)(3(h-1)+1))\right]$$

$$+\frac{|C_1|}{2}\sum_{\substack{e_{2h}=vu\in C_{2h}\\ h=1,\ldots,n+1}}\left[\left(10hm+8h-6m-5\right)\times(3(m+1)(2n+3-2h))+(m+1)(6h-5)\times(10m(n-h)+10m+8(n-h)+8)\right]$$

$$+\frac{|F_1|}{2}\sum_{\substack{f_{3h+1}=vu\in F_{3h+1}\\ h=1,\ldots,n}}\left[\left(10hm+2m+8h+1\right)\times(m+1)(6n-6h+1)\}+(m+1)(6h+3)\times((10m+8)(n-h)+4m+3)\right]$$

$$+\frac{|F_1|}{2}\sum_{\substack{f_{3h}=vu\in F_{3h}\\ h=1,\ldots,n}}\left[\left((10m+8)h-2m-2\right)+(m+1)(6h+3)\times((10m+8)(n-h)+8m+6)\right]$$

$$+\frac{|F_1|}{2}\sum_{\substack{f_{3h-1}=vu\in F_{3h-1}\\ h=1,\ldots,n}}\left[\left(10hm-4m+8h-4\right)\times 3(m+1)(3n+2-2h)+6h(m+1)\times((10m+8)(n-h)+10m+8)\right]$$

$$=\frac{|C_1|}{2}\sum_{\substack{e_{2h-1}=vu\in C_{2h-1}\\ h=1,\ldots,n+1}}\left[120m^2nh-100m^2n-120m^2h^2+264m^2h-136m^2+216mnh\right.$$

$$\left.-180mn-216mh^2+474mh-244m+96nh-80n-96h^2+210h-108\right]$$

$$+\frac{|C_1|}{2}\sum_{\substack{e_{2h}=vu\in C_{2h}\\ h=1,\ldots,n+1}}\left[120m^2nh-86m^2n-120m^2h^2+236m^2h-104m^2+216mnh-156mn\right.$$

$$\left.-216mh^2+426mh-189m+96nh-70n-96h^2+190h-85\right]$$

$$+\frac{|F_1|}{2}\sum_{\substack{f_{3h+1}=vu\in F_{3h+1}\\ h=1,\ldots,n}}\left[120m^2nh+42m^2n-120m^2h^2-8m^2h+14m^2+216mnh+72mn\right.$$

$$\left.-216mh^2-12mh+24m+96nh+30n-96h^2-4h+10\right]$$

$$+\frac{|F_1|}{2}\sum_{\substack{f_{3h}=vu\in F_{3h}\\ h=1,\ldots,n}}\left[60m^2nh+30m^2n-60m^2h^2+18m^2h+24m^2+108mnh+54mn\right.$$

$$\left.-108mh^2+40mh+40m+48nh+24n-48h^2+20h+16\right]$$

$$+\frac{|F_1|}{2}\sum_{\substack{f_{3h-1}=vu\in F_{3h-1}\\ h=1,\ldots,n}}\left[-120h^2m^2-216h^2m-96h^2+150hm^2n+144hm^2+270hmn\right.$$

$$\left.+264hm+120hn+120h-36m^2n-24m^2-72mn-48m-36n-24\right]$$

$$=\frac{(2m+1)}{2}\left[6+14m+8m^2+36mn+15n-mn+20m^2n+144mnn+25n^2\right.$$

$$\left.-87mn^2+32m^2n^2+108mnn^2+16n^3-72mn^3+20m^2n^3\right]$$

$$+\frac{(2m+1)}{2}\left[9+21m+12m^2+60mn+18n-18mn+24m^2n+168mnn\right.$$

$$+25n^2 - 111mn^2 + 32m^2n^2 + 108mnn^2 + 16n^3 - 72mn^3 + 20m^2n^3\big]$$
$$+\frac{2(m+1)}{2}\big[2(-4n - 9mn - 5m^2n + 90mnn + 14n^2 - 57mn^2 + 19m^2n^2 + 54mnn^2 + 8n^3 - 36mn^3 + 10m^2n^3)\big]$$
$$+\frac{2(m+1)}{2}\big[18n + 42mn + 23m^2n + 108mnn + 34n^2 - 34mn^2 + 39m^2n^2 + 54mnn^2 + 8n^3 - 36mn^3 + 10m^2n^3\big]$$
$$+\frac{2(m+1)}{2}\big[20n + 48mn + 28m^2n + 36n^2 + 87mn^2 + 51m^2n^2 + 28n^3 + 63mn^3 + 35m^2n^3\big]$$
$$= \frac{1}{2}\big[15 + 93n + 246n^2 + 136n^3 + 12mn(8 + 74n + 45n^2) + m^2(90 + 232n - 198n^2 - 208n^3) + 2m^3(20 + 85n + 192n^2 + 105n^3) + m(65 + 251n - 24n^2 - 66n^3 + 12mn(16 + 100n + 63n^2))\big]$$

which is the required result.■

[III] CONCLUSION

In this paper, certain degree based topological indices, namely generalized Randić, general Zagreb, general sum-connectivity, ABC, GA; ABC_4 and GA_5 indices for the para-line graphs of ortho-polyphenyl chain, meta-polyphenyl chain and para-polyphenyl chain were studied.

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