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THE EDGE-PADMAKAR-IVAN INDEX OF THE TITANIA NANOTUBES TiO_2 *(m,n)*

Jialin Zheng [1], Mohammad R. Farahani [3], Muhammad K. Jamil [4] Muhammad K. Siddiqui [5] and Xiujun Zhang* [1, 2]

School of Information Science and Engineering [1], Key Laboratory of Pattern Recognition and Intelligent Information Processing Institutions of Higher Education of Sichuan Province [2], Chengdu University, Chengdu, 610106, China.
Department of Applied Mathematics [3], Iran University of Science and Technology (IUST), Narmak, Tehran 16844, Iran.
Department of Mathematics [4], Riphah Institute of Computing and Applied Sciences (RICAS), Riphah International University, Lahore, Pakistan.
Department of Mathematics [5], Comsats Institute of Information Technology, Sahiwal, Pakistan.

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Correspondence to Author:
Xiujun Zhang

School of Information Science and Engineering, Chengdu University, Chengdu, 610106, China.

E-mail: woodszhang@cdu.edu.cn

ABSTRACT: Let *G(V,E)* be a simple connected graph. For an edge *e=uv*, $m_u(e)$ is the number of edges lying closer to the vertex *u* than *v*, analogously define $m_v(e)$. The edge version of *PI* index of a graph *G* is defined as $PI_e(G) = \sum_{e=uv\in E(G)}[m_u(e)+m_v(e)]$.Nano-structured TiO_2 has been widely used in various applications such as biosensors, solar cells and biomaterials. Synthesis of nano-structured Titanium dioxide (TiO_2) such as Nanotubes, Nano-wires and nano-fibers has raised interest lately due to their high surface to volume ratio and the ability of provoke a greater degree of biological plasticity compared to conventional microstructures. Nano-structured TiO_2, has been widely used in various applications such as biosensors, solar cells, photocatalysis, phoelectrolysis and biomaterials. In this paper, we compute the edge-PI index of Titania Nanotubes TiO_2.

INTRODUCTION: Let *G* be a simple connected graph with vertex set *V(G)* and edge set *E(G)*, respectively. The distance between two vertices $u,v\in V(G)$ is defined as the number of edges in a minimal path connecting the vertices *u,v*, and is denoted as *d(u,v)*. If *e=uv*, is an edge and *y* is a vertex of the connected graph *G*, then the distance between *e* and *y* is equal to $\min\{d(u,y),d(v,y)\}$.

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For an edge $e=uv\in E(G)$, $n_u(e)$ is the number of vertices of graph *G* whose distance to the vertex *u* is smaller than the distance to the vertex *v* in *G*; analogously $n_v(e)$ is the number of vertices of *G* whose distance to the vertex *v* in *G* is smaller than the distance to the vertex *u*. Similarly, $m_u(e)$ is the number of edges of *G* whose distance to the vertex *u* is smaller than the distance to the vertex *v*, analogously $m_v(e)$ denotes the number of edges of *G* whose distance to the vertex *v* is smaller than the distance to the vertex *u*.

A topological index is a real number related to a graph. It must be a structural invariant, *i.e.*, it preserves by every graph automorphisms. There are several topological indices have been defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of molecules.

The vertex-PI index was introduced by Ashrafi *et al.*, [1] as:

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

Khadikar *et al.*, [2] introduced the edge-PI index as:

$$PI_e(G) = \sum_{e=uv\in E(G)} [m_u(e) + m_v(e)]$$

The mathematical properties of the *PI* and its applications in chemistry and nano-sciences are well studied for details see [3 - 14].

Synthesis of nano-structured Titanium dioxide (TiO_2) such as Nanotubes, Nano-wires and nano-fibers has raised interest lately due to their high surface to volume ratio and the ability of provoke a greater degree of biological plasticity compared to conventional microstructures. Nano-structured TiO_2, has been widely used in various applications such as biosensors, solar cells, photocatalysis, phoelectrolysis and biomaterials. A 2-dimensional lattice of the Titania Nanotubes, $TiO_2[m,n]$, is shown in **Fig. 1** and for more chemical properties of TiO_2 Nanotubes and TiO_2 nano-composite, see [15- 18]. In $TiO_2[m,n]$, *m* and *n* denotes the number of octagons in a column and the number of octagons in a row [19 - 37]. In this paper, we computed the edge-PI index of the Titania Nanotubes.

RESULTS AND DISCUSSION: In this section, we will compute the edge-PI index of the Titania Nanotubes with the help of cut method and orthogonal cuts [38, 39].

Theorem 1: The edge-PI index of the Titania Nanotubes $TiO_2[m,n]$ $(m,n \geq 1)$ is given by

$$PI_e(TiO_2[m,n]) = 340m^2n + 144m^2 + 362mn + 29m + 216n + 151$$

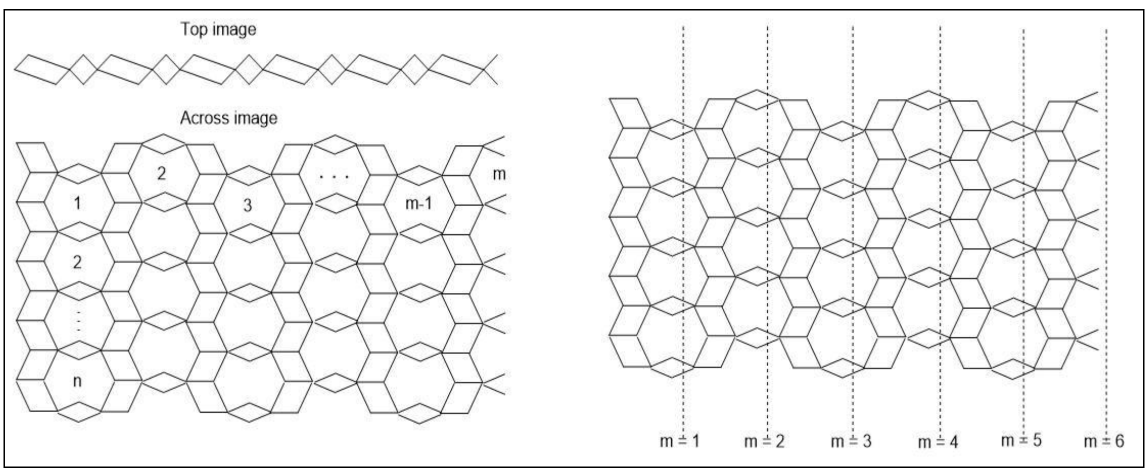

FIG. 1: 2-DIMENSIONAL LATTICE OF THE TITANIA NANOTUBES, $TiO_2[m,n]$

Proof: A graphical representation of Titania Nanotubes $TiO_2[m,n]$ is shown in **Fig. 1**. This graph has $2(3n+2)(m+1)$ vertices and $10mn+6m+8n+4$ edges.

By using the Cut Method and finding Orthogonal Cuts of the Titania Nanotubes $TiO_2(m,n)$, we can determine all edge cuts (quasi-orthogonal) of $TiO_2(m,n)$ and compute all $m_u(e|TiO_2(m,n))$ and $m_v(e|TiO_2(m,n))$, $\forall e \in E(TiO_2(m,n))$.

Here in this paper (see **Fig. 2**) $\forall e=uv \in E(TiO_2(m,n))$, we denote $m_u(e|TiO_2(m,n))$ as the number of edges in the left component of $TiO_2(m,n)-C(e)$ and alternatively $m_v(e|TiO_2(m,n))$ as the number of edges in the right component of $TiO_2(m,n)-C(e)$.

Thus by according to the structure of Titania Nanotubes $TiO_2(m,n)$ in **Fig. 2**, we see that there are $2n+3(n+1)=5n+3$ vertical cuts for all oblique or horizontal edges in $TiO_2(m,n)$, $\forall\ m,n \in \mathbb{N}$ and obviously all these orthogonal cuts are vertical. Now on based an edge e is an oblique edge or a horizontal edge, we denote its orthogonal cut by C_i or F_j for all $i=1,\dots,C=2(n+1)$ and $j=1,\dots, F= 2n+ n+1$ (obviously C+F=$5n+3$).

Again by according to the structure of $TiO_2(m,n)$ in **Fig. 2**, we can see that the size of all orthogonal cuts C_i are equivalence and is $2m+1=|C_i|$ and the size of all orthogonal cuts F_i are equivalence, too, and is $2(m+1)=|F_i|$. Thus for all orthogonal cuts C_i and F_i, we have following results. In case the orthogonal cuts C_i $(i=1,\ldots,2(n+1))$, see **Fig. 2**:

- For C_1: $m_u(e_1|TiO_2(m,n))=0$ and $m_v(e_1|TiO_2(m,n))=|E(TiO_2(m,n))|-|C_1|=10mn+6m+8n+4-(2m+1)=10mn+4m+8n+3$.

- For C_2: $m_u(e_2|TiO_2(m,n))=|C_1|+|F_1|=2m+1+2m+2=4m+3$ and $m_v(e_2|TiO_2(m,n))=|E(TiO_2(m,n))|-(|C_1|+|F_1|+|C_2|)=10mn+6m+8n+4-(6m+4)=10mn+8n$.

- For C_3: $m_u(e_3|TiO_2(m,n))=2|C_1|+3|F_1|=10m+8$ and $m_v(e_3|TiO_2(m,n))=|E(TiO_2(m,n))|-(3|C_1|+3|F_1|)=10mn+6m+8n+4-(12m+9)=10mn+8n-6m-5$.

- For C_4: $m_u(e_4|TiO_2(m,n))=3|C_1|+4|F_1|=14m+11$ and $m_v(e_4|TiO_2(m,n))=|E(TiO_2(m,n))|-(4|C_1|+4|F_1|)=10mn+6m+8n+4-(16m+12)=10mn+8n-10m-8$.

- For $C_{(2h-1)}$:
  $m_u(e_{(2h-1)}|TiO_2(m,n))=(2h-2)|C_1|+(3h-3)|F_1|=(2h-2)(2m+1)+(3h-3)(2m+2)=(10m+8)(h-1)$
  and
  $m_v(e_{(2h-1)}|TiO_2(m,n))=|E(TiO_2(m,n))|-((2h-1)|C_1|+(3h-3)|F_1|)=10mn+6m+8n+4-(10m+8)(h-1)-(2m+1)$

- For $C_{(2h)}$:
  $m_u(e_{(2h)}|TiO_2(m,n))=(2h-1)|C_1|+(3h-2)|F_1|=(2h-1)(2m+1)+(3h-2)(2m+2)=10hm+8h-6m-5$
  and
  $m_v(e_{(2h)}|TiO_2(m,n))=|E(TiO_2(m,n))|-(2h|C_1|+(3h-2)|F_1|)=10m(n-h)+10m+8(n-h)+8$.

- For C_{2n+2}:
  $m_u(e_{2n+2}|TiO_2(m,n))=(2n+1)|C_1|+(3n+1)|F_1|=(2n+1)(2m+1)+(3n+1)(2m+2)=10nm+8n+4m+3$
  and
  $m_v(e_{2n+2}|TiO_2(m,n))=0$.

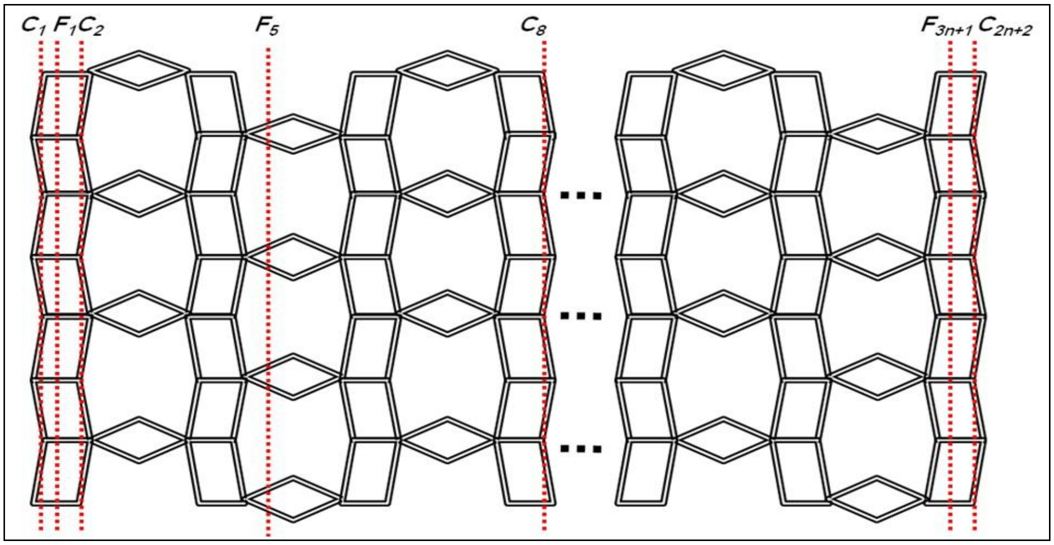

FIG. 2: CUTTING OF EDGES BY ORTHOGONAL CUTS/CUT METHOD OF TITANIA NANOTUBE

In case the orthogonal cuts F_j $(j=1,\ldots,3n+1)$, see **Fig. 2**:

- For F_1: $m_u(e_1|TiO_2(m,n))=2m+1=|C_i|$ and $m_v(e_1|TiO_2(m,n))=|E(TiO_2(m,n))|-(|C_1|+|F_1|)= 10mn+6m+8n+4-(4m+3)=10mn+8n+2m+1$.

- For F_2: $m_u(e_2|TiO_2(m,n))=2|C_1|+|F_1|=6m+4$ and $m_v(e_2|TiO_2(m,n))=|E(TiO_2(m,n))|-(2|C_1|+2|F_1|)=10mn+6m+8n+4-(8m+6)=10mn+8n-2m-2$.

- For F_3: $m_u(e_3|TiO_2(m,n))=2|C_1|+2|F_1|=8m+6$ and $m_v(e_3|TiO_2(m,n))=|E(TiO_2(m,n))|-(2|C_1|+3|F_1|) = 10mn+6m+8n+4-(10m+8)=10mn+8n-4m-4$.

- For F_4: $m_u(e_4|TiO_2(m,n))=3|C_1|+3|F_1|=12m+9$ and $m_v(e_4|TiO_2(m,n))=|E(TiO_2(m,n))|-(3|C_1|+4|F_1|) = 10mn+6m+8n+4-(14m+11)=10mn+8n-8m-7$.

- For F_5: $m_u(e_5|TiO_2(m,n))=4|C_1|+4|F_1|=16m+12$ and $m_v(e_5|TiO_2(m,n))=|E(TiO_2(m,n))|-(4|C_1|+5|F_1|)=10mn+6m+8n+4-(18m+14)=10mn+8n-12m-10$.

- For F_6: $m_u(e_6|TiO_2(m,n))=4|C_1|+5|F_1|=18m+14$ and $m_v(e_6|TiO_2(m,n))=|E(TiO_2(m,n))|-(4|C_1|+6|F_1|)=10mn+6m+8n+4-(20m+16)=10mn+8n-14m-12$.

- For F_7: $m_u(e_7|TiO_2(m,n))=5|C_1|+6|F_1|=22m+17$ and $m_v(e_7|TiO_2(m,n))=|E(TiO_2(m,n))|-(5|C_1|+7|F_1|)=10mn+6m+8n+4-(24m+19)$.

- For F_8: $m_u(e_8|TiO_2(m,n))=6|C_1|+7|F_1|=26m+20$ and $m_v(e_8|TiO_2(m,n))=|E(TiO_2(m,n))|-(6|C_1|+8|F_1|)=10mn+6m+8n+4-(28m+22)$.

- For F_{3h+1} $(h=0,\dots,n)$:
  $m_u(F_{3h+1}|TiO_2(m,n))=(2h+1)|C_1|+(3h)|F_1|=(2h+1)(2m+1)+(3h)(2m+2)=10hm+2m+8h+1$.
  $m_v(F_{3h+1}|TiO_2(m,n))=|E(TiO_2(m,n))|-(10hm+2m+8h+1)=(10m+8)(n-h)+4m+3$.

- For F_{3h-1} $(h=1,\dots,n)$:
  $m_u(F_{3h-1}|TiO_2(m,n))=(2h)|C_1|+(3h-2)|F_1|=(2h)(2m+1)+(3h-2)(2m+2)$
  $=(10m+8)h-2|F_1|=10hm-4m+8h-4$.
  $m_v(F_{3h-1}|TiO_2(m,n))=(10mn+6m+8n+4)-(10hm-4m+8h-4)=(10m+8)(n-h)+10m+8$.

- For F_{3h} $(h=1,\dots,n)$:
  $m_u(F_{3h}|TiO_2(m,n))=m_u(F_{3h-1}|TiO_2(m,n))+|F_1|=2h|C_1|+(3h-1)|F_1|$
  $=(10m+8)h-|F_1|=(10m+8)h-2m-2$.
  $m_v(F_{3h}|TiO_2(m,n))=m_v(F_{3h-1}|TiO_2(m,n))-|F_1|=(10m+8)(n-h)+8m+6$.

Here, we can compute the edge Szeged index of the Titania Nanotubes $TiO_2(m,n)$ $(\forall m,n>1)$ as:

$$PI_e(TiO_2[m,n])=\sum_{e_i=uv\in E(TiO_2(m,n))}(m_u(e_i|TiO_2(m,n))+m_v(e_i|TiO_2(m,n)))$$

$$=\sum_{\substack{e_i=vu\in C_i\\ i=1,\dots,2n+2}}|C_i|\left[m_u\left(e_i|TiO_2(m,n)\right)+m_v\left(e_i|TiO_2(m,n)\right)\right]$$

$$+\sum_{\substack{f_i=vu\in F_i\\ i=1,\dots,3n+1}}|F_i|\left[m_u\left(f_i|TiO_2(m,n)\right)+m_v\left(f_i|TiO_2(m,n)\right)\right]$$

$$=|C_1|\sum_{\substack{e_{2h-1}=vu\in C_{2h-1}\\h=1,\dots,n+1}}\left[m_u\left(e_{2h-1}\mid TiO_2(m,n)\right)+m_v\left(e_{2h-1}\mid TiO_2(m,n)\right)\right]$$
$$+|C_1|\sum_{\substack{e_{2h}=vu\in C_{2h}\\h=1,\dots,n+1}}\left[m_u\left(e_i\mid TiO_{2h}(m,n)\right)+m_v\left(e_{2h}\mid TiO_2(m,n)\right)\right]$$
$$+|F_1|\sum_{\substack{f_{3k+1}=vu\in F_{3k+1}\\k=0,1,\dots,n}}\left[m_u\left(f_{3k+1}\mid TiO_2(m,n)\right)+m_v\left(f_{3k+1}\mid TiO_2(m,n)\right)\right]$$
$$+|F_1|\sum_{\substack{f_{3k}=vu\in F_{3k}\\k=1,\dots,n}}\left[m_u\left(f_{3k}\mid TiO_2(m,n)\right)+m_v\left(f_{3k}\mid TiO_2(m,n)\right)\right]$$
$$+|F_1|\sum_{\substack{f_{3k-1}=vu\in F_{3k-1}\\k=1,\dots,n}}\left[m_u\left(f_{3k-1}\mid TiO_2(m,n)\right)+m_v\left(f_{3k-1}\mid TiO_2(m,n)\right)\right]$$

$$=(2m+1)\begin{bmatrix}(10mn+4m+8n+3)+(14m+11+10mn+8n-6m-5)+\dots+\\((10m+8)(h-1)+10mn+6m+8n+4-(10m+8)(h-1)-(2m+1))\end{bmatrix}+$$
$$(2m+1)\begin{bmatrix}(4m+3+10mn+2m+8n)+(14m+11+10mn+8n-10m-8)+\dots+\\(10hm+8h-6m-5+10m(n-h)+10m+8(n-h)+8)+(10mn+8n+4m+3)\end{bmatrix}+$$
$$2(m+1)\begin{bmatrix}(2m+1+10mn+8n+2m+1)+(12m+9+10mn+8n-8m-7)+\\(22m+17+10mn+6m+8n+4-24m+19)+\dots+\\(10hm+2m+8h+1+(10m+8)(n-h)+4m+3)\end{bmatrix}+$$
$$2(m+1)\begin{bmatrix}(8m+6+10mn+8n-4m-4)+(18m+13+10mn+8n-14m-11)+\dots+\\((10m+8)h-2m-2+(10m+8)(n-h)+8m+6)\end{bmatrix}+$$
$$2(m+1)\begin{bmatrix}(6m+4+10mn+8n-2m-2)+(16m+12+10mn+8n-12m-10)+\dots+\\(10hm-4m+8h-4+(10m+8)(n-h)+10m+8)\end{bmatrix}$$

$$=(2m+1)\left[30mn+16m+24n+11\right]+(2m+1)[40mn+18m+32n+12]+$$
$$2(m+1)[40mn+18m+32n+48]+2(m+1)[30mn+16m+24n+8]+$$
$$2(m+1)[30mn+14m+24n+8]$$
$$=340m^2n+144m^2+362mn+29m+216n+151$$

Which is the required result.

CONCLUSION: In this paper, we computed the closed formulas of the edge-PI index of Titania Nanotubes TiO_2. Nano-structured TiO_2 has been widely used in various applications such as biosensors, solar cells and biomaterials. Synthesis of nano-structured Titanium dioxide (TiO_2) such as Nanotubes, Nano-wires and nano-fibers has raised interest lately due to their high surface to volume ratio and the ability of provoke a greater degree of biological plasticity compared to conventional microstructures. Khadikar *et al.*, proposed a topological index named the edge-PI index (shortly PI_e) as:

$$PI_e(G)=\sum_{e=uv\in E(G)}[m_u(e)+m_v(e)],$$

where $m_u(e)$ is the number of edges of G whose distance to the vertex u is smaller than the distance to the vertex v, analogously $m_v(e)$ denotes the number of edges of G whose distance to the vertex v is smaller than the distance to the vertex u.

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