Research Article

Zafar Hussain, Mobeen Munir*, Muhammad Bilal, Alam Ameer, Shazia Rafique, and Shin Min Kang*

Computational Analysis of new Degree-based descriptors of oxide networks

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Abstract: Oxide networks have diverse applications in the polymer and pharmaceutical industries. Polynomials and degree-based topological indices have tendencies to correlate properties of molecular graphs. In this article, we formulate the closed forms of Zagreb and forgotten polynomials and topological indices such as Hyper-Zagreb index, first and second multiple Zagreb indices, forgotten index, Albert index, Bell index, $IRM(G)$ of oxide networks. We also compute the F-index of complement of oxide networks, F-coindex of G and F-coindex of complement of oxide networks. We put graphical analysis of each index with respect to the parameter involved in each case.

Keywords: Degree-based topological index, Oxide network, Forgotten Index, Co-index

AMS Mathematics Subject Classification: 05C07, 05C10

***Corresponding Author: Mobeen Munir:** Department of Mathematics, Division of Science and Technology, University of Education, Lahore 54000, Pakistan; Email: mmunir@ue.edu.pk

***Corresponding Author: Shin Min Kang:** Department of Mathematics and Research Institute of Natural Science, Gyeongsang National University, Jinju 52828, Korea, and Center for General Education, China Medical University, Taichung 40402, Taiwan; Email: smkang@gnu.ac.kr

Zafar Hussain: Department of Mathematics and Statistics, the University of Lahore, Lahore 54000, Pakistan; Email: hussainzafar888@gmail.com

Muhammad Bilal: Department of Mathematics, The University of Lahore, Gujrat-Pakistan; Email: Muhammad.bilal@mathuol.edu.pk

Alam Ameer: Department of Mathematics, Division of Science and Technology, University of Education, Lahore 54000, Pakistan; Email: alamameer116@yahoo.com

Shazia Rafique: CEMB, University of Punjab, Lahore-Pakistan; Email: shazia.rafiq@ceb.edu.pk

1 Introduction

Today has witnessed the abrupt developments in nano-materials and drugs, which keeps in running with the development of pharmacopodia. The physical and biological testing of new reagents is always a critical issue. In addition, theoretical calculations are performed to model the characteristics of new and proposed compounds to save time and costs. The goal of these calculations is to assist the choice of which compounds to synthesise in the laboratory. One such model which achieved extreme success in recent years, is the graph associated to the underlying compound or structure where every atom is described by a vertex and chemical bond by an edge. Let G be a graph corresponding to the chemical structure with vertex(atom) set $V(G)$ and edge(bond) set $E(G)$. The distance between two vertices u and v is described by $d(u, v)$, is the shortest path between two vertices, similarly the diameter of any graph is the longest distance between any two vertices. The degree of a vertex $v \in V$ is the number of vertices connected to v by edges. The number of vertices in a graph represents its order and the number of edges represents its size. Chemical graph theory, as a branch of mathematical chemistry, attempts to correlate properties of molecular structures using the tools of mathematics like matrices, polynomials, functions and operators. The concept of valence in chemistry is a similar concept to degree of a vertex in graph theory. Graph theory is the branch of mathematics in which the structure of graphs and networks is studied. Graph theory plays a vital role in mathematical chemistry, molecular topology and computational nano-materials [1, 4, 10]. It produces a graph theoretic model of the chemical substance which becomes an entity to be discussed combinatorially and mathematically. Results obtained are checked practically so that properties of the substance under discussion are foreseen.

Chemical graph theory plays substantial role in determining structures and patterns of molecular graphs and networks. With every passing day, new relations between these subjects continue to emerge on the scene. Some basic tools used so far are topological indices and connec-

tivity polynomials in this regard. Attempts are in progress to invent a general polynomial which can provide essential information after application of compositions of several differential and integral operators. Wiener introduced the concept of pass number to measure properties such as heats of formation, chromatographic retention time, boiling point and strain energy [1]. Hosoya introduced the Hosoya index in 1971 and used distance matrix to redefine the pass number (w) of Wiener [2]. Since Wiener's definition was useful only for acyclic molecular graphs, it did not capture the attention of chemists, nevertheless Hosoya's paper made it popular. Hosoya's other substantial contribution appeared in 1988 to define w by proposing Wiener polynomial, which, is now known as Hosoya polynomial [3]. Distance based polynomials and functions are invariants of the structures and preserve the metric structure.

In the context of degree-based indices, a recent good addition is the M-polynomial that plays exactly the same role in parallel to the Hosoya polynomial for distance-based indices [5]. In [6–9, 11, 12], several authors used the M-polynomial and related topological indices of different structures involving nanostar dendrimers, polyhex nanotubes, hex-derived networks, and some benzenoid systems. In fact the M-polynomial and other related polynomials like Zagreb and Forgotten polynomials are studied relatively more than other polynomials. Topological index preserves the topological symmetries of the structure and are frequently used in quantitative structure-activity relationships (QSARs). Here these indices are used to predict toxicity and determine regularity decisions, risk assessment, drug discovery and lead optimization [2, 4, 13, 14]. Researchers are actively working to discover new polynomials and topological indices and their actual correlations of these indices and properties of the chemical structures and nano-materials.

In the present work, we present new topological characterizations of oxide networks in the form of degree-based indices and polynomials. Moreover we also compute co-indices of these networks. We also determine the closed forms of some indices which determine the irregularity of oxide networks. For basic preliminaries and introductory literature review we refer [34, 35] and references therein.

2 Main Results

In this part we establish our new results about oxide networks, (OX_n) , $n > 1$. This network can be obtained by removing all silicon nodes from silicone network of dimension

n , [15, 16]. Figure 1 is a schematic illustration of an oxide network of dimension 5.

Figure 1: Figure of (OX_5)

We reserve the symbol (OX_n) , $n > 1$ for oxide network of dimension n . From figures (1-2) it is obvious that the order and size of (OX_n) is respectively, $9n^2 + 3n$ and $18n^2$. Another noticeable observation is the fact that (OX_n) , $n > 1$ has only vertices of degree 2 and 4. In this paper we compute first Zagreb polynomial, second Zagreb polynomial, Forgotten polynomial and some topological indices such as Hyper-Zagreb index, first and second multiple Zagreb indices, Forgotten index, Albert index, Bell index, $IRM(G)$ and $M_1(L(G))$. We also compute first and second Zagreb coindices, F-index of complement of (OX_n) , F-coindex of (OX_n) and F-coindex of complement of oxide networks. We also give graphical analysis of each index and co-index with respect to the parameters involved in each class.

The following result gives the general form of Zagreb Polynomials and Forgotten polynomial of the oxide networks.

Theorem 2.1. *Let (OX_n) , $n > 1$ be oxide network. Then first Zagreb polynomial, second Zagreb polynomial and Forgotten polynomial of (OX_n) are*

- $M_1(OX_n; x) = 12nx^6 + (18n^2 - 12n)x^8$,
- $M_2(OX_n; x) = 12nx^8 + (18n^2 - 12n)x^{16}$,
- $F(OX_n; x) = 12nx^{20} + (18n^2 - 12n)x^{32}$.

Proof. Let (OX_n) , $n > 1$ is oxide network having order $n = 9n^2 + 3n$ and size $m = 18n^2$. From figure 1–2, we come

to know that the oxide networks (OX_n) has only vertices of degree 2 and 4. Let V_1 and V_2 represent vertices of degree 2 and 4 respectively, where $|V_1| = 6n$ and $|V_2| = 9n^2 - 3n$. The edge partitions of (OX_n) are

$E_{\{2,4\}} = e = uv \in E(OX_n) / d_u = 2, d_v = 4 \rightarrow |E_{\{2,4\}}| = 12n$,
 $E_{\{4,4\}} = e = uv \in E(OX_n) / d_u = 4, d_v = 4 \rightarrow |E_{\{4,4\}}| = 18n^2 - 12n$, where $E_{\{2,4\}}$ is the set of edges having end vertices of degree 2 and 4 and $E_{\{4,4\}}$ is the set of edges having end vertices of degree 4 and 4.

a. By definition the first Zagreb polynomial,

$$\begin{aligned} M_1(OX_n, x) &= \sum_{uv \in E(OX_n)} x^{[d_u + d_v]}, \\ &= \sum_{uv \in E_1(OX_n)} x^{[d_u + d_v]} + \sum_{uv \in E_2(OX_n)} x^{[d_u + d_v]} \\ &= |E_1(OX_n)|x^6 + |E_2(OX_n)|x^8 \\ &= 12nx^6 + (18n^2 - 12n)x^8. \end{aligned}$$

b. Now by definition the second Zagreb polynomial,

$$\begin{aligned} M_2(OX_n, x) &= \sum_{uv \in E(OX_n)} x^{[d_u \times d_v]}, \\ &= \sum_{uv \in E_1(OX_n)} x^{[d_u \times d_v]} + \sum_{uv \in E_2(OX_n)} x^{[d_u \times d_v]}, \\ &= |E_1(OX_n)|x^8 + |E_2(OX_n)|x^{16} \\ &= 12x^8 + (18n^2 - 12n)x^{16}, \end{aligned}$$

c. Now by definition the Forgotten polynomial,

$$\begin{aligned} F(OX_n; x) &= \sum_{uv \in E(OX_n)} x^{[d_u^2 + d_v^2]}, \\ &= \sum_{uv \in E_1(OX_n)} x^{[d_u^2 + d_v^2]} + \sum_{uv \in E_2(OX_n)} x^{[d_u^2 + d_v^2]}, \\ &= |E_1(OX_n)|x^{20} + |E_2(OX_n)|x^{32}, \\ &= 12nx^{20} + (18n^2 - 12n)x^{32}. \end{aligned}$$

Theorem 2.2. Let $OX_n, n > 1$ is oxide networks. Then

- $HM(OX_n) = 1152n^2 - 336n$,
- $PM_1(OX_n) = 3^{12n} \cdot 2^{54n^2 - 24n}$,
- $PM_2(OX_n) = 2^{72n^2 - 12n}$,
- $F(OX_n) = 576n^2 - 144n$.

Proof. a. By definition of hyper-Zagreb index

$$\begin{aligned} HM(OX_n) &= \sum_{uv \in E(OX_n)} [d_u + d_v]^2, \\ &= \sum_{uv \in E_1(OX_n)} [d_u + d_v]^2 + \sum_{uv \in E_2(OX_n)} [d_u + d_v]^2, \\ &= 36|E_1(OX_n)| + 64|E_2(OX_n)|, \\ &= 1152n^2 - 336n. \end{aligned}$$

b. By the definition of first Zagreb index,

$$\begin{aligned} PM_1(OX_n) &= \prod_{uv \in E(OX_n)} [d_u + d_v], \\ &= \prod_{uv \in E_1(OX_n)} [d_u + d_v] \times \prod_{uv \in E_2(OX_n)} [d_u + d_v], \\ &= 6^{|E_1(OX_n)|} \times 8^{|E_2(OX_n)|}, \\ &= 3^{12n} \times 2^{54n^2 - 24n}, \end{aligned}$$

c. By definition of second multiple Zagreb index,

$$\begin{aligned} PM_2(OX_n) &= \prod_{uv \in E(OX_n)} [d_u \times d_v], \\ &= \prod_{uv \in E_1(OX_n)} [d_u \times d_v] \times \prod_{uv \in E_2(OX_n)} [d_u \times d_v], \\ &= 8^{|E_1(OX_n)|} \times 16^{|E_2(OX_n)|}, \\ &= 2^{72n^2 - 12n}, \end{aligned}$$

d. By definition of Forgotten index,

$$\begin{aligned} F(OX_n) &= \sum_{uv \in E(OX_n)} [d_u^2 + d_v^2], \\ &= \sum_{uv \in E_1(OX_n)} [d_u^2 + d_v^2] + \sum_{uv \in E_2(OX_n)} [d_u^2 + d_v^2], \end{aligned}$$

$$\begin{aligned} &= 20|E_1(OX_n)| + 32|E_2(OX_n)|, \\ &= 576n^2 - 144n. \end{aligned}$$

□

Theorem 2.3. Let (OX_n), $n > 1$ is oxide network, then

- Albertson index, $A(OX_n) = 24n$,
- Bell index, $B(OX_n) = \frac{24n(3n-1)}{(3n+1)}$,
- IRM(OX_n) = 48n,
- $M_1(L(OX_n)) = 24n(27n - 10)$.

Proof. a. **Albertson index**

$$\begin{aligned} A(OX_n) &= \sum_{xy \in E(OX_n)} |d(x) - d(y)|, \\ &= \sum_{xy \in E_1(OX_n)} |d(x) - d(y)| + \sum_{xy \in E_2(OX_n)} |d(x) - d(y)|, \\ &= |E_1(OX_n)||2 - 4| + |E_2(OX_n)||4 - 4|, \\ &= (12n)(2) + (18n^2 - 12n)(0), \\ &= 24n, \end{aligned}$$

b. **Bell Index**

$$\begin{aligned} B(OX_n) &= \sum_{x \in V(OX_n)} (d(x) - \frac{2m}{n})^2, \\ &= \sum_{x \in V_1(OX_n)} (d(x) - \frac{2m}{n})^2 + \sum_{x \in V_2(OX_n)} (d(x) - \frac{2m}{n})^2, \\ &= |V_1(OX_n)|(2 - \frac{2(18n^2)}{9n^2 + 3n})^2 + |V_2(OX_n)|(4 - \frac{2(18n^2)}{9n^2 + 3n})^2, \\ &= 6n(2 - \frac{2(18n^2)}{9n^2 + 3n})^2 + (9n^2 - 3n)(4 - \frac{2(18n^2)}{9n^2 + 3n})^2, \\ &= \frac{24n(3n-1)}{3n+1}, \end{aligned}$$

c. **IRM(G)**

$$\begin{aligned} \square \quad IRM(OX_n) &= \sum_{xy \in E(OX_1)} [d(x) - d(y)]^2, \\ &= \sum_{xy \in E_1(OX_1)} [d(x) - d(y)]^2 + \sum_{xy \in E_2(OX_1)} [d(x) - d(y)]^2, \\ &= |E_1(OX_n)||2 - 4|^2 + |E_2(OX_n)||4 - 4|^2, \\ &= (12n)(-2)^2 + (18n^2 - 12n)(0)^2, \\ &= 48n, \end{aligned}$$

d. $M_1(L(G))$

$$\begin{aligned} M_1(L(G)) &= \sum_{xy \in E(G)} [d(x) + d(y) - 2]^2, \\ M_1(L(OX_n)) &= \sum_{xy \in E_1(OX_n)} [d(x) + d(y) - 2]^2 + \\ &\quad \sum_{xy \in E_2(OX_n)} [d(x) + d(y) - 2]^2, \\ &= |E_1(OX_n)||2 + 4 - 2|^2 + |E_2(OX_n)||4 + 4 - 2|^2, \\ &= (12n)(4)^2 + (18n^2 - 12n)(6)^2, \\ &= 24n(27n - 10). \end{aligned}$$

□

Theorem 2.4. Let oxide network (OX_n), $n > 1$ then,

- $\overline{M}_1(G) = 12n(27n^3 - 3n^2 - 3n + 2)$,
- $\overline{M}_2(G) = 26n(18n^3 - 10n + 3)$.

Proof. Let oxide network (OX_n), $n > 1$ having order $n = 9n^2 + 3n$ and size $m = 18n^2$, the first Zagreb index $M_1(OX_n)$ of (OX_n) is $144n^2 - 24n$ and the second Zagreb index $M_2(OX_n)$ of oxide network is $288n^2 - 96n$ then,

a. $\overline{M}_1(G)$,

$$\begin{aligned} \overline{M}_1(G) &= 2m(n - 1) - M_1(G), \\ \overline{M}_1(OX_n) &= 2(18n^2)(9n^2 + 3n - 1) - (144n^2 - 24n), \\ &= 12n(27n^3 - 3n^2 - 3n + 2), \end{aligned}$$

b. $\overline{M}_2(G)$

$$\overline{M}_2(G) = 2m^2 - \frac{1}{2}M_1(G) - M_2(G),$$

$$\overline{M_2}(OX_n) = 2(18n^2)^2 - \frac{1}{2}(144n^2 - 24n) - (288n^2 - 96n), \\ = 26n(18n^3 - 10n + 3). \quad \square$$

Theorem 2.5. Let oxide network (OX_n) , $n > 1$, then,

$$a. \overline{F}(OX_n) = 3n(486n^7 + 1782n^6 + 81n^5 - 2286n^4 + 1485n^3 + 459n^2 - 438n + 71),$$

$$b. \overline{F}(OX_n) = 24n(54n^3 + 9n^2 - 33n + 7),$$

$$c. \overline{F}(OX_n) = 12n(54n^5 + 162n^4 - 243n^3 - 54n^2 + 87n - 12),$$

Proof. Let oxide network (OX_n) , $n > 1$ having order $n = 9n^2 + 3n$ and size $m = 18n^2$, the first zagreb index $M_1(OX_n)$ of (OX_n) is $144n^2 - 24n$ and the Forgotten index $F(OX_n)$ of oxide network is $576n^2 - 144n$, then

a. $\overline{F}(OX_n)$

$$F(\overline{G}) = n(n-1)^3 - 6m(n-1)^2 + 3(n-1)M_1(G) - F(G),$$

$$F(\overline{OX_n}) = (9n^2 + 3n)(9n^2 + 3n - 1)^3 - 6(18n^2)(9n^2 + 3n - 1)^2 + 3(9n^2 + 3n - 1)(144n^2 - 24n) - (576n^2 - 144n),$$

$$F(\overline{OX_n}) = 3n(486n^7 + 1782n^6 + 81n^5 - 2286n^4 + 1485n^3 + 459n^2 - 438n + 71), \quad b. \overline{F}(OX_n)$$

$$\overline{F}(G) = (n-1)M_1(G) - F(G),$$

$$\overline{F}(OX_n) = (9n^2 + 3n - 1)(144n^2 - 24n) - (576n^2 - 144n),$$

$$\overline{F}(OX_n) = 24n(54n^3 + 9n^2 - 33n + 7),$$

c. $\overline{F}(OX_n)$

$$\overline{F}(G) = 2m(n-1)^2 - 2(n-1)M_1(G) + F(G),$$

$$\overline{F}(OX_n) = 2(18n^2)(9n^2 + 3n - 1)^2 - 2(9n^2 + 3n - 1)(144n^2 - 24n) + (576n^2 - 144n),$$

$$\overline{F}(OX_n) = 12n(54n^5 + 162n^4 - 243n^3 - 54n^2 + 87n - 12). \quad \square$$

$PM_1(OX_n)$ remains negligible for $n \leq 4$. After $n > 5$ it rises without bounds. It is evident from Figure 7 that $PM_2(OX_n)$ remains negligible for $n \leq 3$. After $n > 4$ it rises without bounds. The shape of the graph of $F(OX_n)$ is a parabola, showing that it increases rapidly with an increase in n , Figure 8.

Figure 2: Graphs of Zagreb and Forgotten indices

3 Computational Analysis and Description

In this part we give computational analysis of computed indices of oxide networks. Figure 2 gives dependence of M_1 , M_2 and F on the involved parameter n . Clearly, Forgotten index increases sharply as compared to M_1 , and M_2 . However these three indices increase with increase in n . It is now an established fact that total π -electron energy is related with Forgotten index [4, 10], so it can be concluded that this energy will rise with the rise in n . Figure 3 suggests that Bell, Albertson and IRM are linearly related with n . However Bell index is the slowest in these indices. All these three indices actually measure the tendency of structure to be irregular. These graphs show that the oxide network becomes more irregular and complex as n increases. Figure 4 suggests that first Zagreb index of the line graph of oxide networks is linearly related with n . The graph in Figure 5 shows the dependence of $HM(OX_n)$ on n . It is clear that this index is more sensitive than the above described indices for large range of n . It is evident from Figure 6 that

Figure 3: Graphs of Albertson, Bell, and IRM indices

Figure 4: Graph of first Zagreb index of line graph

Figure 7: Graph of $PM_2(OX_n)$ Figure 5: Graph of $HM(OX_n)$ Figure 8: Graph of $F(OX_n)$ Figure 6: Graph of $PM_1(OX_n)$

4 Conclusions

M-polynomial and other related polynomials such as Zagreb and Forgotten polynomials have recently been studied in a high frequency. In [34], the authors computed degree-based indices of alpha boron nanotubes and compared the behaviour of these indices on two types of boron nanotubes. In [35], Hussain et al. formulated degree-based indices and co-indices of honey-comb networks. The present article provides computation of several indices and co-indices of oxide networks. In particular, we computed Forgotten and Zagreb polynomials of general oxide networks. We also provided index analysis of oxide networks and dependence of these indices in the form of graphs using Mapple. These indices are actually correlated with chemical properties of oxide networks and will be useful for people practically working in chemical industry.

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