Research Article

Computing Some Degree-Based Topological Indices of Honeycomb Networks

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A topological index is a numeric quantity related with the chemical composition claiming to correlate the chemical structure with different chemical properties. Topological indices serve to predict physicochemical properties of chemical substance. Among different topological indices, degree-based topological indices would be helpful in investigating the anti-inflammatory activities of certain chemical networks. In the current study, we determine the neighborhood second Zagreb index and the first extended first-order connectivity index for oxide network (OX_n), silicate network (SL_n), chain silicate network (CS_n), and hexagonal network (HX_n). Also, we determine the neighborhood second Zagreb index and the first extended first-order connectivity index for honeycomb network (HC_n).

1. Introduction

Chemical graph theory/mathematical chemistry has made easier for the scientists to predict physicochemical properties of different chemical structures using topological indices. A numeric value assigned to a molecular graph (a graph portraying chemical compounds) is recognized as the topological index, and it remains unchanged under the isomorphism of the graph. For a given period, there is an increasing interest in topological indices that reflect some structural features of molecular compounds. Topological indices hold attention because they correlate well with certain chemical properties of molecular graphs. Also, they play an important role in the quantitative structure-activity relationship (QSAR) and quantitative structure property relationship (QSPR) studies [1]. To overview the structure-activity relationship, topological indices are required to effectively characterize structural features and bioactivity of chemical compounds [2–4]. In the current study, under

discussion, molecular structures are nanostructures due to their design and applications.

All the graphs in present study are simple, undirected, finite, and connected. For a vertex $w \in V(G)$, we use the notation $N(w)$ for the set containing the vertices adjacent to w . The degree of a vertex w is the cardinality of the set $N(w)$ and is denoted by d_w . Let $\mathcal{S}(w)$ denote the sum of degrees of the vertices adjacent to w . In other words, $\mathcal{S}(w) = \sum_{uw \in E(G)} d_u$ and $N(t) = \{v \in V(G) \mid tv \in E(G)\}$. For undefined terminologies related to graph theory, the author can read [5–7]. Consider the following general graph invariant:

$$I(G) = \sum_{vw \in E(G)} f(\mathcal{S}(v), \mathcal{S}(w)). \quad (1)$$

Some special cases of the above invariants I have already been appeared in mathematical chemistry. For example, if we take $f(\mathcal{S}(v), \mathcal{S}(w)) = \mathcal{S}(v)\mathcal{S}(w)$ or $1/\sqrt{\mathcal{S}(v)\mathcal{S}(w)}$,

then I gives neighborhood second Zagreb index NM_2 [8] and the first extended first-order connectivity index ${}^1\chi_1$ [9, 10], respectively. These indices are defined as

$${}^1\chi_1(G) = \sum_{vw \in E(G)} \frac{1}{\sqrt{S(v)S(w)}}, \quad (2)$$

$$NM_2(G) = \sum_{vw \in E(G)} \mathcal{S}(v)\mathcal{S}(w). \quad (3)$$

Toropov et al. [11] proved that extended molecular connectivity indices have good correlation with the boiling point of chemical structures. Detail about theoretical and computation aspects of some families of chemical structures can be viewed in [12–16].

In this report, we are interested in five well-known chemical structures, name as oxide network (OX_n), honeycomb network (HC_n), silicate network (SL_n), chain silicate network (CS_n), and hexagonal network (HX_n). As far as authors are aware, neighborhood second Zagreb index and the first extended first-order connectivity index of oxide network (OX_n), silicate network (SL_n), chain silicate network (CS_n), hexagonal network (HX_n), and honeycomb network (HC_n) have not been investigated until now, and therefore, the study under consideration is an addition in the aforesaid direction.

2. Motivation

Since topological indices are useful to predict the physico-chemical properties of chemical compounds, therefore, it is important to analyze the correlation of the topological indices investigated. Yousaf et al. [17] proved that the correlation of entropy and eccentric factor of octane isomers with neighborhood second Zagreb index and the first extended first-order connectivity index has high accuracy. In addition, topological indices are moreover used for discrimination against octane isomers. The discrimination ability of an index has remarkable application within the coding and the computer processing of molecular structures (isomers).

Denote by $x_{q,r}(H)$ (or $x_{q,r}$, when terms are not confusing) the number of edges in H with end-vertex degrees q and r . Two graphs H_1 and H_2 are called edge-equivalent graphs if they are satisfying $x_{q,r}(H_1) = x_{q,r}(H_2)$ for all q and r with $1 \leq q \leq r \leq \Delta$. A topological index TI is called edge-equivalent topological index if it satisfies $TI(H_1) = TI(H_2)$ for every pair of edge-equivalent graphs H_1 and H_2 . We notice that the bond incident degree indices [18, 19] (BID indices for short [20]) are edge-equivalent topological indices. General form of the BID indices is

$$BID(H) = \sum_{vw \in E(G)} g(d_v, d_w) = \sum_{q \leq r} x_{q,r} g(q, r). \quad (4)$$

where $g(q, r)$ is a bivariate symmetric function. It is worth noting that most of the degree-based topological indices used in mathematical chemistry are BID indices. These indices may be produced from equation (4) based on the selection of $g(q, r)$.

To study the discriminatory performance of the topological index NM_2 and ${}^1\chi_1$, the class of octane isomers are considered which are representing the 8-vertex trees. These 18 molecular graphs of octane isomers are shown in Figure 1. Figure 1 makes it easy to see that trees O_3 and O_4 are edge-equivalent, but their corresponding first extended first-order connectivity indices and neighborhood second Zagreb indices are not the same: ${}^1\chi_1(O_3) = 0.097$, ${}^1\chi_1(O_4) = 0.096$, $NM_2(O_3) = 106$, and $NM_2(O_4) = 107$. Similarly, the trees O_{11} and O_{12} are edge-equivalent graphs possessing different first extended first-order connectivity indices and neighborhood second Zagreb indices: ${}^1\chi_1(O_{11}) = 0.086$, ${}^1\chi_1(O_{12}) = 0.087$, $NM_2(O_{13}) = 136$, and $NM_2(O_4) = 137$.

Thus, the topological index NM_2 and ${}^1\chi_1$ does not belong to the class of edge-equivalent topological indices. Subsequently, we can presume that the topological indices NM_2 and ${}^1\chi_1$ are identified by a better discriminatory power than the conventional BID indices. Particularly, Wang et al. [21] proved that all the molecular graphs of 18 octane isomers have different NM_2 and ${}^1\chi_1$ values. It is worth mentioning that, in certain specific cases, the discriminatory capacity of NM_2 and ${}^1\chi_1$ is limited, but still better than that of the BID indices. This can be explained by examining the corresponding edge-equivalent graphs illustrated in Figure 2: we have $NM_2(D_1) = 451$ and ${}^1\chi_1(D_1) = 1.09$, but $NM_2(D_2) = NM_2(D_3) = 448$ and ${}^1\chi_1(D_2) = {}^1\chi_1(D_3) = 1.08$ (of course, these three graphs are identical for any arbitrary BID index; in other words, with the help of an arbitrary BID index, it is difficult to distinguish between the graphs D_1 , D_2 , and D_3).

3. Main Results and Discussion

Multiprocessor interconnection networks are frequently needed to join many identical processor-memory pairs that are repeated, each one is referred to as a processing node. Message passing rather than shared memory is frequently used for synchronization of a communication between the processing nodes for the execution of the program. Multiprocessor interconnection networks are most attracted networks due to the accessibility of powerful and inexpensive microprocessors and memory chips. By repeating regular polygons, periodic plane tessellations can be easily built. For direct interconnection networks, this design is very important as it offers high global performance. Some parallel networks that originate from popular meshes are silicate, chain silicate, hexagonal, honeycomb, and oxide networks. Such networks have very attractive topological properties that have been investigated in various ways in [22–33].

3.1. Oxide Networks. Oxide networks are important in investigating silicate networks. Oxide networks are obtained by the deletion of silicon nodes from a silicate network (see Figure 3). An oxide network of dimension n is denoted as OX_n . The order and size of OX_n is $9n^2 + 3n$ and $18n^2$, respectively. In oxide networks OX_n , the edge set can be partitioned into six sets depending on degree summation of neighbors of end vertices. This partition is presented in Table 1.

FIGURE 1: Graphs of octane isomers. (a) O_1 . (b) O_2 . (c) O_3 . (d) O_4 . (e) O_5 . (f) O_6 . (g) O_7 . (h) O_8 . (i) O_9 . (j) O_{10} . (k) O_{11} . (l) O_{12} . (m) O_{13} . (n) O_{14} . (o) O_{15} . (p) O_{16} . (q) O_{17} . (r) O_{18} .

FIGURE 2: Edge-equivalent graphs. (a) D_1 . (b) D_2 . (c) D_3 .

FIGURE 3: An oxide network OX_2 .

TABLE 1: Edge partitions of OX_n .

$(S(v)S(w))$, where $vw \in E(OX_n)$	Cardinality
(8, 12)	12
(12, 14)	12
(16, 16)	$18n^2 - 36n + 18$
(8, 1)	$12(n - 1)$
(14, 16)	$12(n - 1)$
(14, 14)	$6(2n - 3)$

In the following theorems, we investigate ${}^1\chi_1$ and NM_2 of OX_n .

Theorem 1. The ${}^1\chi_1$ index of oxide networks OX_n is given by

$${}^1\chi_1(OX_n) = \frac{9}{8}n^2 + \left(\frac{3}{\sqrt{7}} + \frac{3}{\sqrt{14}} - \frac{39}{28}\right)n + \frac{3}{\sqrt{6}} - \frac{3}{\sqrt{7}} + \frac{6}{\sqrt{42}} - \frac{3}{\sqrt{14}} - \frac{9}{56}. \quad (5)$$

Proof. We use equation (2) and Table 1 to calculate the expression for ${}^1\chi_1$ index of the oxide networks OX_n :

$$\begin{aligned} {}^1\chi_1(OX_n) &= \sum_{vw \in E(G)} \frac{1}{\sqrt{\mathcal{S}(v)\mathcal{S}(w)}} \\ &= (12) \frac{1}{\sqrt{8 \times 12}} + (12) \frac{1}{\sqrt{12 \times 14}} \\ &\quad + 12(n-1) \frac{1}{\sqrt{8 \times 14}} + 6(2n-3) \frac{1}{\sqrt{14 \times 14}} \\ &\quad + 12(n-1) \frac{1}{\sqrt{14 \times 16}} \\ &\quad + (18n^2 - 36n + 18) \frac{1}{\sqrt{16 \times 16}} \\ &= \frac{9}{8}n^2 + \left(\frac{3}{\sqrt{7}} + \frac{3}{\sqrt{14}} - \frac{39}{28}\right)n \\ &\quad + \frac{3}{\sqrt{6}} - \frac{3}{\sqrt{7}} + \frac{6}{\sqrt{42}} - \frac{3}{\sqrt{14}} - \frac{9}{56}. \end{aligned} \quad (6)$$

□

Theorem 2. The NM_2 index of oxide networks OX_n is given by

$$NM_2(OX_n) = 4608n^2 - 2832n + 216. \quad (7)$$

Proof. To calculate the expression for neighborhood second Zagreb index of oxide networks OX_n , we use equation (3) and Table 1 to get the required result:

$$\begin{aligned} NM_2(OX_n) &= \sum_{vw \in E(G)} \mathcal{S}(v)\mathcal{S}(w) \\ &= (12)(8 \times 12) + (12)(12 \times 14) \\ &\quad + 6(2n-3)(14 \times 14) + 12(n-1)(8 \times 14) \\ &\quad + (18n^2 - 36n + 18)(16 \times 16) \\ &\quad + 12(n-1)(14 \times 16) \\ &= 4608n^2 - 2832n + 216. \end{aligned} \quad (8)$$

□

3.2. Honeycomb Networks. In material sciences, honeycomb networks have vital role in different fields especially in computer graphics, cellular phone base stations, and image processing and in representing benzenoid hydrocarbons. Honeycomb networks are shaped by the iterative use of hexagonal tiles in a specific design. We denote the n -dimensional honeycomb network with n hexagons between central and boundary hexagon by HC_n . HC_n is constructed by adding layer of hexagon around HC_{n-1} (see Figure 4). The order and size of HC_n is $6n^2$ and $9n^2 - 3n$, respectively. Table 2 shows partition of edges.

By using partition of edges of HC_n , we investigate ${}^1\chi_1$ and NM_2 of HC_n in the following theorems.

Theorem 3. The ${}^1\chi_1$ index of Honeycomb network HC_n is given by

$${}^1\chi_1(HC_n) = n^2 + \left(\frac{2}{\sqrt{7}} + \frac{12}{\sqrt{35}} - \frac{7}{3}\right)n + \frac{38}{15} - \frac{12}{\sqrt{35}} - \frac{2}{\sqrt{7}}. \quad (9)$$

Proof. We use equation (2) and Table 2 to calculate the expression for ${}^1\chi_1$ index of the Honeycomb network HC_n :

$$\begin{aligned} {}^1\chi_1(HC_n) &= \sum_{vw \in E(G)} \frac{1}{\mathcal{S}(v)\mathcal{S}(w)} \\ &= (6) \frac{1}{\sqrt{5 \times 5}} + 12(n-1) \frac{1}{\sqrt{5 \times 7}} + 6(n-1) \frac{1}{\sqrt{7 \times 9}} + (9n^2 - 21n + 12) \frac{1}{\sqrt{9 \times 9}} \\ &= n^2 + \left(\frac{2}{\sqrt{7}} + \frac{12}{\sqrt{35}} - \frac{7}{3}\right)n + \frac{38}{15} - \frac{12}{\sqrt{35}} - \frac{2}{\sqrt{7}}. \end{aligned} \quad (10)$$

□

FIGURE 4: Honeycomb network.

TABLE 2: Edge partitions of HC_n .

$(S(v)S(w))$, where $vw \in E(HC_n)$	Cardinality
(5, 5)	6
(5, 7)	$12(n - 1)$
(7, 9)	$6(n - 1)$
(9, 9)	$9n^2 - 21n + 12$

Theorem 4. *The NM_2 index of Honeycomb network HC_n is given by*

$$NM_2(HC_n) = 729n^2 - 903n + 324. \quad (11)$$

Proof. To calculate the expression for NM_2 index of Honeycomb network HC_n , we use equation (3) and Table 2, to get the required result:

$$\begin{aligned}
 NM_2(HC_n) &= \sum_{vw \in E(G)} \mathcal{S}(v)\mathcal{S}(w) \\
 &= (6)(5 \times 5) + 12(n - 1)(5 \times 7) \\
 &\quad + 6(n - 1)(7 \times 9) + (9n^2 - 21n + 12)(9 \times 9) \\
 &= 729n^2 + 903n + 324.
 \end{aligned} \quad (12)$$

□

3.3. Silicate Networks. Silicates are constituent elements of the common minerals that form the rock and, absolutely,

the most important and the most complicated minerals. The elementary unit of silicates' minerals are tetrahedron SiO_4 . Silicate is produced by melting metal oxides or metal sand carbonates. SiO_4 tetrahedral content is nearly found in all silicate materials. A silicate sheet is formed by different types of sequences of tetrahedrons which are connected by adjoining oxygen vertices to other tetrahedrons in a plane. Cyclic silicates are networks that result in rings of different lengths after being bound by sharing oxygen vertices. Figures 5 and 6 present certain cyclic and sheet silicates, respectively. Other types of silicates are also available and are illustrated in Figure 7. From a chemical perspective, the oxygen atoms are in fact the corner vertices of tetrahedron SiO_4 and silicon atom is its central vertex. Graphically, we describe the central atom as silicon vertex, corner atoms as oxygen vertices, and edges are bonds between them. Figure 8 illustrates a tetrahedron of SiO_4 . We denote a silicate array with n hexagons between center and border of silicate sheet by SL_n . Figure 9 illustrates a three-dimensional silicate network. The order and size of SL_n is $15n^2 + 3n$ and $36n^2$, respectively. In the following theorems, the silicate networks are analyzed through certain graph invariants.

In the next theorem, we computed ${}^1\chi_1$ and NM_2 of the SL_n in the following way.

Theorem 5. *The ${}^1\chi_1$ index of silicate networks is given by*

$$\begin{aligned}
 {}^1\chi_1(SL_n) &= \left(\frac{3}{\sqrt{15}} + \frac{3}{5} \right) n^2 + \left(\frac{8}{3\sqrt{5}} + \frac{4}{3\sqrt{6}} - \frac{5}{\sqrt{15}} + \frac{4}{3\sqrt{10}} - \frac{16}{45} \right) n \\
 &\quad + \frac{4}{\sqrt{10}} - \frac{8}{3\sqrt{5}} - \frac{4}{3\sqrt{6}} + \frac{2}{\sqrt{15}} + \frac{2}{3\sqrt{2}} - \frac{4}{3\sqrt{10}} - \frac{1}{15}.
 \end{aligned} \quad (13)$$

FIGURE 5: Cyclic silicates.

FIGURE 6: Sheet silicates.

FIGURE 7: (a) Ortho, (b) pyro, and (c) chain silicates.

FIGURE 8: SiO_4 tetrahedron.

FIGURE 9: For $n = 3$, silicate network SL_n .

Proof. We use equation (2) and Table 3 to calculate the expression for ${}^1\chi_1$ index of the silicate networks:

$$\begin{aligned}
 {}^1\chi_1(SL_n) &= \sum_{vw \in E(G)} \frac{1}{\sqrt{\mathcal{S}(v)\mathcal{S}(w)}} \\
 &= (6n) \frac{1}{\sqrt{15 \times 15}} + (24) \frac{1}{\sqrt{15 \times 24}} + 24(n-1) \frac{1}{\sqrt{15 \times 27}} + 12(n-1) \frac{1}{\sqrt{18 \times 27}} \\
 &\quad + (18n^2 - 30n + 12) \frac{1}{\sqrt{18 \times 30}} + (12) \frac{1}{\sqrt{24 \times 27}} + 6(2n-3) \frac{1}{\sqrt{27 \times 27}} \\
 &\quad + 12(n-1) \frac{1}{\sqrt{27 \times 30}} + (18n^2 - 36n + 18) \frac{1}{\sqrt{30 \times 30}} \\
 &= \frac{2n}{5} + \frac{4}{\sqrt{10}} + \frac{8(n-1)}{3\sqrt{5}} + \frac{4(n-1)}{3\sqrt{6}} + \frac{6n^2 - 10n + 4}{2\sqrt{15}} + \frac{2}{3\sqrt{2}} + \frac{2(2n-3)}{9} \\
 &\quad + \frac{4(n-1)}{3\sqrt{10}} + \frac{6n^2 - 12n + 6}{10} \\
 &= \left(\frac{3}{\sqrt{15}} + \frac{3}{5} \right) n^2 + \left(\frac{8}{3\sqrt{5}} + \frac{4}{3\sqrt{6}} - \frac{5}{\sqrt{15}} + \frac{4}{3\sqrt{10}} - \frac{16}{45} \right) n \\
 &\quad + \frac{4}{\sqrt{10}} - \frac{8}{3\sqrt{5}} - \frac{4}{3\sqrt{6}} + \frac{2}{\sqrt{15}} + \frac{2}{3\sqrt{2}} - \frac{4}{3\sqrt{10}} - \frac{1}{15}.
 \end{aligned} \tag{14}$$

Theorem 6. The NM_2 index of silicate networks is given by

$$NM_2(SL_n) = 25920n^2 - 13230n + 702. \tag{15}$$

Proof. To calculate the expression for NM_2 index of silicate networks, we use equation (3) and Table 3 to get the required result:

$$\begin{aligned}
 NM_2(SL_n) &= \sum_{vw \in E(G)} \mathcal{S}(v)\mathcal{S}(w) \\
 &= (6n)(15 \times 15) + 12(n-1)(18 \times 27) \\
 &\quad + (24)(15 \times 24) \\
 &\quad + 12(n-1)(27 \times 30) + 24(n-1)(15 \times 27) \\
 &\quad + (18n^2 - 30n + 12)(18 \times 30)
 \end{aligned} \quad \square$$

TABLE 3: Edge partition of LS_n .

$(S(v)S(w))$, where $vw \in E(LS_n)$	Cardinality
(15, 15)	$6n$
(18, 27)	$12(n-1)$
(27, 30)	$12(n-1)$
(18, 30)	$18n^2 - 30n + 12$
(15, 27)	$24(n-1)$
(24, 27)	12
(15, 24)	24
(27, 27)	$6(2n-3)$
(30, 30)	$18n^2 - 36n + 18$

$$\begin{aligned}
& + (12)(24 \times 27) + 6(2n-3)(27 \times 27) \\
& + (18n^2 - 36n + 18)(30 \times 30) \\
& = 25920n^2 - 13230n + 702.
\end{aligned} \tag{16}$$

FIGURE 10: n -dimensional chain silicate network.

3.4. Chain Silicate Networks. Chain silicate is acquired by linear arrangement of tetrahedron. n -dimensional chain silicate networks are characterized as follows. A network of n -dimensional chain silicate stands for CS_n is acquired by linear arrangement of n tetrahedron. The order and size of CS_n with $n > 1$ is $3n + 1$ and $6n$, respectively. A network of n -dimensional chain silicate is illustrated in Figure 10.

Tables 4 and 5 suggest such a partition that we use to compute certain topological indices. Now, within the following theorems, we analyzed the chain silicate networks CS_n via topological indices.

$$\begin{aligned}
{}^1\chi_1(CS_3) &= \sum_{vw \in E(G)} \frac{1}{\sqrt{\mathcal{S}(v)\mathcal{S}(w)}} \\
&= (6) \frac{1}{\sqrt{12 \times 12}} + (1) \frac{1}{\sqrt{15 \times 15}} + (6) \frac{1}{\sqrt{12 \times 21}} + (1) \frac{1}{\sqrt{21 \times 21}} + (4) \frac{1}{\sqrt{15 \times 21}} \\
&= \frac{1}{2} + \frac{1}{15} + \frac{1}{\sqrt{7}} + \frac{1}{21} + \frac{4}{\sqrt{315}}.
\end{aligned} \tag{17}$$

The following results provide the investigation of certain topological indices of CS_n .

Theorem 7. The ${}^1\chi_1$ index of CS_n is given by

$${}^1\chi_1(CS_n) = \begin{cases} \frac{1}{2} + \frac{1}{\sqrt{6}} & \text{if } n = 2, \\ \frac{1}{2} + \frac{1}{15} + \frac{1}{\sqrt{7}} + \frac{1}{21} + \frac{4}{\sqrt{315}} & \text{if } n = 3, \\ \left(\frac{13}{120} + \frac{2}{3\sqrt{10}} \right) n + \frac{1}{5} + \frac{1}{\sqrt{7}} - \frac{2}{\sqrt{10}} + \frac{4}{\sqrt{315}} + \frac{1}{\sqrt{126}} & \text{if } n > 3. \end{cases} \tag{18}$$

TABLE 4: Edge partition of CS_n .

$(S(v)S(w))$, where $vw \in E(CS_n)$	Cardinality
(12, 12)	6
(12, 21)	6
(15, 15)	$n - 2$
(15, 21)	4
(15, 24)	$4n - 12$
(21, 24)	2
(24, 24)	$n - 4$

TABLE 5: Edge partition of CS_3 .

$(S(v)S(w))$, where $vw \in E(CS_3)$	Cardinality
(12, 12)	6
(15, 15)	1
(12, 21)	6
(15, 21)	4
(21, 21)	1

Proof. There are three cases that need to be examined in order to prove these outcomes. First, we demonstrate this

$$\begin{aligned}
{}^1\chi_1(CS_3) &= \sum_{vw \in E(G)} \frac{1}{\sqrt{\mathcal{S}(v)\mathcal{S}(w)}} \\
&= (6) \frac{1}{\sqrt{12 \times 12}} + (1) \frac{1}{\sqrt{15 \times 15}} + (6) \frac{1}{\sqrt{12 \times 21}} + (1) \frac{1}{\sqrt{21 \times 21}} + (4) \frac{1}{\sqrt{15 \times 21}} \\
&\quad + 4(n-3) \frac{1}{\sqrt{15 \times 24}} + (2) \frac{1}{\sqrt{21 \times 24}} + (n-4) \frac{1}{\sqrt{24 \times 24}} \\
&= \left(\frac{13}{120} + \frac{2}{3\sqrt{10}} \right) n + \frac{1}{5} + \frac{1}{\sqrt{7}} - \frac{2}{\sqrt{10}} + \frac{4}{\sqrt{315}} + \frac{1}{\sqrt{126}}.
\end{aligned} \tag{20}$$

Theorem 8. The NM_2 index of the chain silicate networks CS_n is given by

$$NM_2(CS_n) = \begin{cases} 2160 & \text{if } n = 2, \\ 4302 & \text{if } n = 3, \\ 2241n - 2430 & \text{if } n > 3. \end{cases} \tag{21}$$

Proof. There are three cases that need to be examined in order to prove these outcomes. First, we demonstrate this result for $n = 2$. In the graph $G = CS_2$, the edge partition is of the type $(\mathcal{S}(12), \mathcal{S}(12))$ and $(\mathcal{S}(12), \mathcal{S}(18))$ and each of this partition has six edges. Then,

$$\begin{aligned}
NM_2(CS_2) &= \sum_{vw \in E(G)} \mathcal{S}(v)\mathcal{S}(w) \\
&= (6)(12 \times 12) + (6)(12 \times 18) \\
&= 2160.
\end{aligned} \tag{22}$$

For the case $n = 3$, the edge partition CS_n is presented in Table 5. Now, $NM_2(CS_3)$ can be computed as

result for $n = 2$. In the graph $G = CS_2$, the edge partition is of the type $(\mathcal{S}(12), \mathcal{S}(12))$ and $(\mathcal{S}(12), \mathcal{S}(18))$ and each of this partition has six edges. Then,

$$\begin{aligned}
{}^1\chi_1(CS_2) &= \sum_{vw \in E(G)} \frac{1}{\sqrt{\mathcal{S}(v)\mathcal{S}(w)}} \\
&= (6) \frac{1}{\sqrt{12 \times 12}} + (6) \frac{1}{\sqrt{12 \times 18}} \\
&= \frac{1}{2} + \frac{1}{\sqrt{6}}.
\end{aligned} \tag{19}$$

For the case $n = 3$, the edge partition CS_n is presented in Table 5. Now, ${}^1\chi_1(CS_3)$ can be computed as follows:

Let us now turn to the third case of $n > 3$. To calculate the expression for ${}^1\chi_1$ index of the chain silicate networks CS_n , we use equation (2) and Table 4 to obtain the required result:

$$\begin{aligned}
NM_2(CS_3) &= \sum_{vw \in E(G)} \mathcal{S}(v)\mathcal{S}(w) \\
&= (6)(12 \times 12) + (1)(15 \times 15) + (6)(12 \times 21) \\
&\quad + (1)(21 \times 21) + (4)(15 \times 21) \\
&= 4302.
\end{aligned} \tag{23}$$

Let us now turn to the third case of $n > 3$. To calculate the expression for the NM_2 index of the chain silicate networks CS_n , we use equation (3) and Table 4 to obtain the required result:

$$\begin{aligned}
NM_2(CS_n) &= \sum_{vw \in E(G)} \mathcal{S}(v)\mathcal{S}(w) \\
&= (6)(12 \times 12) + (6)(12 \times 21) + (4)(15 \times 21) \\
&\quad + (n-2)(15 \times 15) \\
&\quad + 4(n-3)(15 \times 24) + (n-4)(24 \times 24) + (2)(21 \times 24) \\
&= 2241n - 2430.
\end{aligned} \tag{24}$$

□

3.5. Hexagonal Networks. It is a known fact that tiling a plane by regular polygon can be done only with regular triangles, hexagons, and squares. A hexagonal network can be obtained by using triangles (see Figure 11). A hexagonal network with n vertices in each side of the hexagon is denoted by HX_n . Let $n > 1$; then, order and size of HX_n is $3n^2 - 3n + 1$ and $9n^2 - 15n + 6$, respectively. Figure 11 depicts the graph of HX_6 . Tables 6–8 depict a partition that we

use to compute the topological indices of hexagonal networks HX_n for $n \geq 3$. Now, we investigate aforementioned indices of hexagonal networks HX_n .

In the following theorems, we investigate ${}^1\chi_1$ and NM_2 of HX_n .

Theorem 9. The ${}^1\chi_1$ index of hexagonal networks HX_n is given by

$${}^1\chi_1(HX_n) = \begin{cases} \frac{3}{5} + \frac{1}{\sqrt{5}} & \text{if } n = 2, \\ \frac{2}{\sqrt{7}} + \frac{6}{\sqrt{406}} + \frac{4}{\sqrt{58}} + \frac{2}{\sqrt{29}} & \text{if } n = 3, \\ \frac{1}{3} + \frac{6}{19} + \frac{1}{\sqrt{8}} + \frac{1}{\sqrt{29}} + \frac{3}{\sqrt{38}} + \frac{3}{\sqrt{58}} + \frac{12}{\sqrt{266}} + \frac{6}{\sqrt{406}} + \frac{12}{\sqrt{551}} & \text{if } n = 4, \\ \left(\frac{1}{4}\right)n^2 + \left(\frac{1}{\sqrt{8}} + \frac{3}{2\sqrt{10}} - \frac{669}{720}\right)n - \frac{1}{4} - \frac{3}{\sqrt{8}} - \frac{6}{\sqrt{10}} + \frac{1}{\sqrt{29}} + \frac{3}{\sqrt{38}} \\ + \frac{3}{\sqrt{58}} + \frac{6}{\sqrt{95}} + \frac{12}{\sqrt{266}} + \frac{6}{\sqrt{406}} + \frac{12}{\sqrt{551}} & \text{if } n > 4. \end{cases} \quad (25)$$

Proof. There are four cases that need to be examined in order to prove these outcomes. First, we demonstrate this result for $n = 2$. In the graph $G = HX_2$, the edge partition is of the type $(\mathcal{S}(10), \mathcal{S}(10))$ and $(\mathcal{S}(10), \mathcal{S}(18))$ and each of this partition has six edges. Then,

$$\begin{aligned} {}^1\chi_1(HX_2) &= \sum_{vw \in E(G)} \frac{1}{\sqrt{\mathcal{S}(v)\mathcal{S}(w)}} \\ &= (6) \frac{1}{\sqrt{10 \times 10}} + (6) \frac{1}{\sqrt{10 \times 18}} \\ &= \frac{3}{5} + \frac{1}{\sqrt{5}}. \end{aligned} \quad (26)$$

For the case $n = 3$, the edge partition HX_3 is presented in Table 6. Now, ${}^1\chi_1(HX_3)$ can be computed as

$$\begin{aligned} {}^1\chi_1(HX_3) &= \sum_{vw \in E(G)} \frac{1}{\sqrt{\mathcal{S}(v)\mathcal{S}(w)}} \\ &= (12) \frac{1}{\sqrt{14 \times 18}} + (6) \frac{1}{\sqrt{14 \times 29}} + (12) \frac{1}{\sqrt{18 \times 29}} \\ &\quad + (12) \frac{1}{\sqrt{29 \times 36}} \\ &= \frac{2}{\sqrt{7}} + \frac{6}{\sqrt{406}} + \frac{4}{\sqrt{58}} + \frac{2}{\sqrt{29}} \end{aligned} \quad (27)$$

For the case $n = 4$, the edge partition HX_4 is presented in Table 7. Now, ${}^1\chi_1(HX_4)$ can be computed as

$$\begin{aligned} {}^1\chi_1(HX_4) &= \sum_{vw \in E(G)} \frac{1}{\sqrt{\mathcal{S}(v)\mathcal{S}(w)}} \\ &= (12) \frac{1}{\sqrt{14 \times 19}} + (6) \frac{1}{\sqrt{19 \times 19}} + (6) \frac{1}{\sqrt{14 \times 29}} \\ &\quad + (12) \frac{1}{\sqrt{19 \times 29}} \\ &\quad + (12) \frac{1}{\sqrt{19 \times 32}} + (12) \frac{1}{\sqrt{29 \times 32}} + (6) \frac{1}{\sqrt{29 \times 36}} \\ &\quad + (12) \frac{1}{\sqrt{32 \times 36}} + (12) \frac{1}{\sqrt{36 \times 36}} \\ &= \frac{1}{3} + \frac{6}{19} + \frac{1}{\sqrt{8}} + \frac{1}{\sqrt{29}} + \frac{3}{\sqrt{38}} + \frac{3}{\sqrt{58}} + \frac{12}{\sqrt{266}} \\ &\quad + \frac{6}{\sqrt{406}} + \frac{12}{\sqrt{551}}. \end{aligned} \quad (28)$$

FIGURE 11: For $n = 6$, hexagonal network HX_n .

Let us now turn to the case of $n > 4$. To calculate the expression for ${}^1\chi_1$ index of hexagonal networks HX_n , we use equation (2) and Table 8 to obtain the required result:

$$\begin{aligned}
 {}^1\chi_1(HX_n) &= \sum_{vw \in E(G)} \frac{1}{\sqrt{\mathcal{S}(v)\mathcal{S}(w)}} \\
 &= (12) \frac{1}{\sqrt{14 \times 19}} + (12) \frac{1}{\sqrt{19 \times 20}} + 6(n-5) \frac{1}{\sqrt{20 \times 20}} + (12) \frac{1}{\sqrt{19 \times 29}} \\
 &\quad + (12) \frac{1}{\sqrt{19 \times 32}} + 12(n-4) \frac{1}{\sqrt{20 \times 32}} + (6) \frac{1}{\sqrt{14 \times 29}} + (12) \frac{1}{\sqrt{29 \times 32}} \\
 &\quad + (6) \frac{1}{\sqrt{29 \times 36}} + 12(n-3) \frac{1}{\sqrt{32 \times 36}} + 6(n-4) \frac{1}{\sqrt{32 \times 32}} \\
 &\quad + (9n^2 - 51n + 72) \frac{1}{\sqrt{36 \times 36}} \\
 &= \left(\frac{1}{4}\right)n^2 + \left(\frac{1}{\sqrt{8}} + \frac{3}{2\sqrt{10}} - \frac{669}{720}\right)n - \frac{1}{4} - \frac{3}{\sqrt{8}} - \frac{6}{\sqrt{10}} + \frac{1}{\sqrt{29}} + \frac{3}{\sqrt{38}} \\
 &\quad + \frac{3}{\sqrt{58}} + \frac{6}{\sqrt{95}} + \frac{12}{\sqrt{266}} + \frac{6}{\sqrt{406}} + \frac{12}{\sqrt{551}}.
 \end{aligned} \tag{29}$$

□

Theorem 10. The NM_2 index of the hexagonal networks HX_n is given by

$$NM_2(HX_n) = \begin{cases} 1680, & \text{if } n = 2, \\ 24252, & \text{if } n = 3, \\ 68478, & \text{if } n = 4, \\ 11664n^2 - 36048n + 26040, & \text{if } n > 4. \end{cases} \tag{30}$$

TABLE 6: Edge partitions of HX_3 .

$(\mathcal{S}(v)\mathcal{S}(w))$, where $vw \in E(HX_3)$	Cardinality
(14, 18)	12
(14, 29)	6
(18, 29)	12
(29, 36)	12

TABLE 7: Edge partitions of HX_4 .

$(\mathcal{S}(v)\mathcal{S}(w))$, where $vw \in E(HX_4)$	Cardinality
(14, 19)	12
(19, 19)	6
(14, 29)	6
(19, 29)	12
(19, 32)	12
(29, 32)	12
(29, 36)	6
(32, 36)	12
(36, 36)	12

Proof. There are four cases that need to be examined in order to prove these outcomes. First, we demonstrate this result for $n = 2$. In the graph $G = HX_2$, the edge partition is of the type $(\mathcal{S}(10), \mathcal{S}(10))$ and $(\mathcal{S}(10), \mathcal{S}(18))$ and each of this partition has six edges. Then,

For the case $n = 3$, the edge partition HX_n is presented in Table 6. Now, $NM_2(HX_3)$ can be computed as

TABLE 8: Edge partitions of HX_n .

$(S(v)S(w))$, where $vw \in E(HX_n)$	Cardinality
(14, 19)	12
(19, 20)	12
(20, 20)	$6(n-5)$
(14, 29)	6
(19, 29)	12
(19, 32)	12
(20, 32)	$12(n-4)$
(29, 32)	12
(29, 36)	6
(32, 32)	$6(n-4)$
(32, 36)	$12(n-3)$
(36, 36)	$9n^2 - 51n + 72$

$$\begin{aligned}
 NM_2(HX_3) &= \sum_{vw \in E(G)} \frac{1}{\sqrt{\mathcal{S}(v)\mathcal{S}(w)}} \\
 &= (12)(14 \times 18) + (6)(14 \times 29) \\
 &\quad + (12)(18 \times 29) + (12)(29 \times 36) \\
 &= 24252.
 \end{aligned} \tag{31}$$

$$\begin{aligned}
 NM_2(HX_n) &= \sum_{vw \in E(G)} \frac{1}{\sqrt{\mathcal{S}(v)\mathcal{S}(w)}} \\
 &= (12)(14 \times 19) + (12)(19 \times 20) + 6(n-5)(20 \times 20) + (12)(19 \times 29) \\
 &\quad + (12)(19 \times 32) + 12(n-4)(20 \times 32) + (6)(14 \times 29) + (12)(29 \times 32) \\
 &\quad + (6)(29 \times 36) + 12(n-3)(32 \times 36) + 6(n-4)(32 \times 32) \\
 &\quad + (9n^2 - 51n + 72)(36 \times 36) \\
 &= 11664n^2 - 36048n + 26040.
 \end{aligned} \tag{32}$$

□

4. Conclusion

The aim of this paper is to discuss the degree-based topological indices of several nanotube networks. In this paper, we determined the neighborhood second Zagreb index and the first extended first-order connectivity index for oxide network (OX_n), silicate network (SL_n), chain silicate network (CS_n), and hexagonal network (HX_n). Also, we determined the neighborhood second Zagreb index and the first extended first-order connectivity index for honeycomb network (HC_n). In this paper, results achieved demonstrate the promising opportunities to apply for chemical sciences. It is very helpful to know more about nanotube networks that have become the central interest of fundamental sciences and study their topological indices that will be completely useful to understand their underlying topologies.

Data Availability

No data were used to support the findings of the study.

For the case $n = 4$, the edge partition HX_n is presented in Table 7. Now, $NM_2(HX_3)$ can be computed as

$$\begin{aligned}
 NM_2(HX_4) &= \sum_{vw \in E(G)} \frac{1}{\sqrt{\mathcal{S}(v)\mathcal{S}(w)}} \\
 &= (12)(14 \times 19) + (6)(19 \times 19) + (6)(14 \times 29) \\
 &\quad + (12)(19 \times 29) \\
 &\quad + (12)(19 \times 32) + (12)(29 \times 32) + (6)(29 \times 36) \\
 &\quad + (12)(32 \times 36) + (12)(36 \times 36) \\
 &= 68478.
 \end{aligned} \tag{32}$$

Let us now turn to the third case of $n > 4$. To calculate the expression for NM_2 index of hexagonal networks HX_n , we use equation (3) and Table 8 to obtain the required result:

Conflicts of Interest

On behalf of all authors, the corresponding author states that there are no conflicts of interest.

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