Biointerface Research in Applied Chemistry
Platinum Open Access Journal (ISSN: 2069-5837)

*Article*
**Volume 11, Issue 5, 2021, 13681 - 13694**
https://doi.org/10.33263/BRIAC115.1368113694

# Neighbourhood Degree - Based Topological Indices of Graphene Structure

**Vignesh Ravi [1], Kalyani Desikan [1,*]**

[1] Division of Mathematics, Vellore Institute of Technology, Chennai; rvignesh.2018@vitstudent.ac.in (R.V.), kalyanidesikan@vit.ac.in (K.D.);
* Correspondence: kalyanidesikan@vit.ac.in;

Scopus Author ID 7005615253

**Received: 8.01.2021; Revised: 7.02.2021; Accepted: 11.02.2021; Published: 14.02.2021**

**Abstract:** The theory of chemical reaction networks is a branch of mathematics that aims to mimic real-world behavior. This research area has drawn many researchers' attention, primarily due to its biological and empirical chemistry applications. The fascinating problems that emerge from the mathematical structures involved have kindled the interest of pure mathematicians. In this paper, we estimate a few topological indices such as SK index, SK1 index, SK2 index, Modified Randić index, and Inverse Sum Index for the Graphene structure based on the neighborhood degree and obtain results based on both sum and products of the cardinality of edge partitions corresponding to 4 different Graphene structures. We also present the 3D representations of the indices using MATLAB.

**Keywords:** graphene; SK; SK1; SK2; Modified Randić Index; Inverse Sum Index.



## 1. Introduction

Chemical reaction network theory is a field of applied mathematics that aims to mimic real-world chemical structure-activity. It has gained an increasing scientific community following since its start in the 19th century, predominantly because of organic chemistry and theoretical chemistry developments. It has also received much attention from pure mathematicians because of the computational design problems that have emerged. Cheminformatics is an active research area where quantitative structure behavior and structure-property relations predict nanomaterial biological activities and properties [1 - 4]. A few physicochemical characteristics and topological indices have been used in research findings to predict organic molecules' bioactivity [5-7].

In a chemical graph, vertices represent atoms or molecules, and edges represent the atoms or molecules' chemical bonding. The degree of a vertex represents the number of edges that are incident on that vertex [8]. The maximum degree in any chemical graph is 4. The notion of a degree in graph theory is closely (but not identically) related to the concept of valency in chemistry.

Graphene is an allotrope of carbon molecules that are constructed on a honeycomb grid (hexagonal pattern). Graphene is the most durable compound material. It has good heat and electric conductive strength. In comparison with graphite, its magnetic property is high and nonlinear.

Topological indices are numerical parameters associated with a graph that characterize its topology. These indices are usually graphed invariant. The topology of chemical structures is described by these indices. The neighborhood degree of a node $a \in V$, indicated as $\delta(a)$ / $\delta_a$, is the sum of degrees of all adjacent nodes of the node $a$. Here, the neighboring nodes of a node are the set of nodes at a distance 1 to the node.

Many researchers [9 - 35] have defined and estimated topological indices of molecules such as graphene, graphene transformations, and their applications.

This paper estimates a few topological descriptors like SK, SK1, SK2 indices, Modified Randić index, and Inverse Sum Index based on the neighborhood degree and obtain results based on both sum and products the cardinality of edge partitions corresponding to 4 different Graphene structures. We also present the 3D representations of the indices using MATLAB.

We define a few new neighborhood degree-based topological indices denoted as $SK_N^{\zeta}(\mathrm{G})$, $SK1_N^{\zeta}(\mathrm{G})$, $SK2_N^{\zeta}(\mathrm{G})$, $mR_N^{\zeta}(\mathrm{G})$, $ISI_N^{\zeta}(\mathrm{G})$ as follows:

$$SK_N^{\zeta}(\mathrm{G}) = \sum_{uv \in E(G)} \left[\frac{\delta(u)+\delta(v)}{2}\right] \quad (1)$$

$$SK1_N^{\zeta}(G) = \sum_{uv \in E(G)} \left[\frac{\delta(u) * \delta(v)}{2}\right] \quad (2)$$

$$SK2_N^{\zeta}(\mathrm{G}) = \sum_{uv \in E(G)} \left[\frac{\delta(u)+\delta(v)}{2}\right]^2 \quad (3)$$

$$mR_N^{\zeta}(\mathrm{G}) = \sum_{uv \in E(G)} \left[\frac{1}{max\{\delta(u),\delta(v)\}}\right] \quad (4)$$

$$ISI_N^{\zeta}(\mathrm{G}) = \sum_{uv \in E(G)} \left[\frac{\delta(u) * \delta(v)}{\delta(u) + \delta(v)}\right] \quad (5)$$

where $\delta(u) = \sum_{v \in N(u)} deg(v)$, $N(u)$ is the Neighborhood set of the vertex $u$.

Figures 1 - 4 shows the structure of graphene.

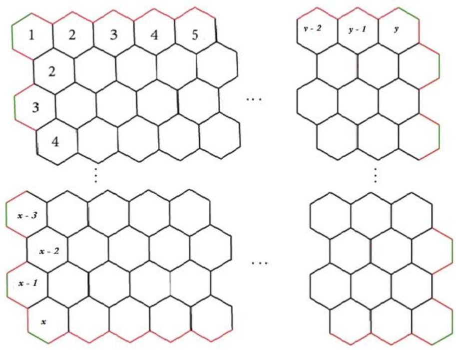


**Figure 1.** Graphene when x > 1 and y > 1.

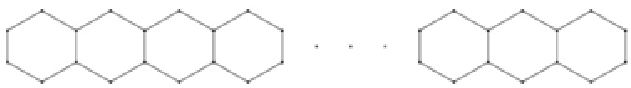

**Figure 2.** Graphene when x = 1 and y > 1.

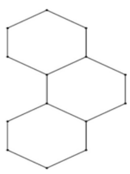

**Figure 3.** Graphene when x > 1 and y = 1.

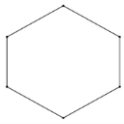

**Figure 4.** Graphene when x = 1 and y = 1.

The edges of graphene can be partitioned into 4 types depending on the number of layers and the number of benzene rings, taking into consideration the neighborhood degrees of the vertices of each edge denoted by $'E_{(\delta(u),\delta(v))}$ / $'E_{(\delta_u,\delta_v)}$. The edge partitions are given in the following tables :

**Table 1.** ΄Edge Partition when x > 1 y > 1.

| $'E_{(\delta_u,\delta_v)}$ | **(4, 5)** | **(5, 5)** | **(5, 7)** | **(5, 8)** | **(6, 7)** | **(7, 9)** | **(8, 8)** | **(8, 9)** | **(9, 9)** |
|---|---|---|---|---|---|---|---|---|---|
| $\lvert 'E_{(\delta_u,\delta_v)}\rvert$ | 4 | x | 8 | 2x-4 | 4y- 8 | 2y | x-2 | 2x-4 | 3xy - 4x - 4y + 5 |

**Table 2.** ΄Edge Partition when x = 1 y > 1.

| $'E_{(\delta_u,\delta_v)}$ | **(4, 4)** | **(4, 5)** | **(5, 7)** | **(6, 7)** | **(7, 7)** |
|---|---|---|---|---|---|
| $\lvert 'E_{(\delta_u,\delta_v)}\rvert$ | 2 | 4 | 4 | 4y - 8 | y - 1 |

**Table 3**. ΄Edge Partition when x > 1 y = 1.

| $'E_{(\delta_u,\delta_v)}$ | **(4, 4)** | **(4, 5)** | **(5, 5)** | **(5, 7)** | **(5, 8)** | **(7, 8)** | **(8, 8)** |
|---|---|---|---|---|---|---|---|
| $\lvert 'E_{(\delta_u,\delta_v)}\rvert$ | 2 | 4 | x - 2 | 4 | 2x - 4 | 2 | 2x - 5 |

**Table 4.** ΄Edge Partition when x = 1 y = 1.

| $'E_{(\delta_u,\delta_v)}$ | **(4, 4)** |
|---|---|
| $\lvert 'E_{(\delta_u,\delta_v)}\rvert$ | 6 |

## 2. Materials and Methods

Our main computational results include the neighborhood degree-based topological indices of graphene structure. We computed the results with the help of the edge partition method and graph-theoretical concepts. The results are depicted graphically using MATLAB 2019 in Figures 5 – 14.

## 3. Results and Discussion

Theorem 2.1: The $SK_N^{\zeta}(G)$ index of graphene with x rows and y benzene rings is

$$SK_N^{\zeta} = \begin{cases} 39x - 38y + 27xy - 57 & if\ x > 1, y > 1 \\ 33y + 39 & if\ x = 1, y > 1 \\ 34x - 11 & if\ x > 1, y = 1 \\ 24 & if\ x = 1, y = 1 \end{cases}$$

Proof: We establish the proof for the following four cases:

Case 1: We use the edge partition for *x > 1, y > 1* given Table 1 in equation 1 and obtain,

$$SK_N^{\zeta} = \lvert 'E_{(4,5)}\rvert \left[\frac{9}{2}\right] + \lvert 'E_{(5,5)}\rvert \left[\frac{10}{2}\right] + \lvert 'E_{(5,7)}\rvert \left[\frac{12}{2}\right] + \lvert 'E_{(5,8)}\rvert \left[\frac{13}{2}\right] + \lvert 'E_{(6,7)}\rvert \left[\frac{13}{2}\right] + \lvert 'E_{(7,9)}\rvert \left[\frac{16}{2}\right] + \lvert 'E_{(8,8)}\rvert \left[\frac{16}{2}\right] + \lvert 'E_{(8,9)}\rvert \left[\frac{17}{2}\right] + \lvert 'E_{(9,9)}\rvert \left[\frac{18}{2}\right]$$

$$= 4\left[\frac{9}{2}\right] + x\left[\frac{10}{2}\right] + 8\left[\frac{12}{2}\right] + (2x - 4)\left[\frac{13}{2}\right] + (4y - 8)\left[\frac{13}{2}\right] + (2y)\left[\frac{16}{2}\right] + (x - 2)\left[\frac{16}{2}\right] + (2x - 4)\left[\frac{17}{2}\right] + (3xy - 4x - 4y + 5)\left[\frac{18}{2}\right]$$

= 39x − 38y + 27xy − 57.

Case 2: Using the edge partition for $x = 1, y > 1$ given in Table 2 in equation 1 we obtain,

$$SK_N^{\zeta} = |'E_{(4,4)}| \left[\frac{8}{2}\right] + |'E_{(4,5)}| \left[\frac{9}{2}\right] + |'E_{(5,7)}| \left[\frac{12}{2}\right] + |'E_{(6,7)}| \left[\frac{13}{2}\right] + |'E_{(7,7)}| \left[\frac{14}{2}\right]$$

$$= 2\left[\frac{8}{2}\right] + 4\left[\frac{9}{2}\right] + 4\left[\frac{12}{2}\right] + (4y - 8)\left[\frac{13}{2}\right] + (y - 1)\left[\frac{14}{2}\right]$$

= 33y + 39.

Case 3: Using the edge partition for $x > 1, y = 1$ given in Table 3 in equation 1 we obtain,

$$SK_N^{\zeta} = |'E_{(4,4)}| \left[\frac{8}{2}\right] + |'E_{(4,5)}| \left[\frac{9}{2}\right] + |'E_{(5,5)}| \left[\frac{10}{2}\right] + |'E_{(5,7)}| \left[\frac{12}{2}\right] + |'E_{(5,8)}| \left[\frac{13}{2}\right] + |'E_{(7,8)}| \left[\frac{15}{2}\right] + |'E_{(8,8)}| \left[\frac{16}{2}\right]$$

$$= 2\left[\frac{8}{2}\right] + 4\left[\frac{9}{2}\right] + (x - 2)\left[\frac{10}{2}\right] + 4\left[\frac{12}{2}\right] + (2x - 4)\left[\frac{13}{2}\right] + 2\left[\frac{15}{2}\right] + (2x - 5)\left[\frac{16}{2}\right]$$

= 34x - 11.

Case 4: Using the edge partition for $x = 1, y = 1$given in Table 4 in equation 1 we obtain,

$$SK_N^{\zeta} = |'E_{(4,4)}| \left[\frac{8}{2}\right]$$

= 24.

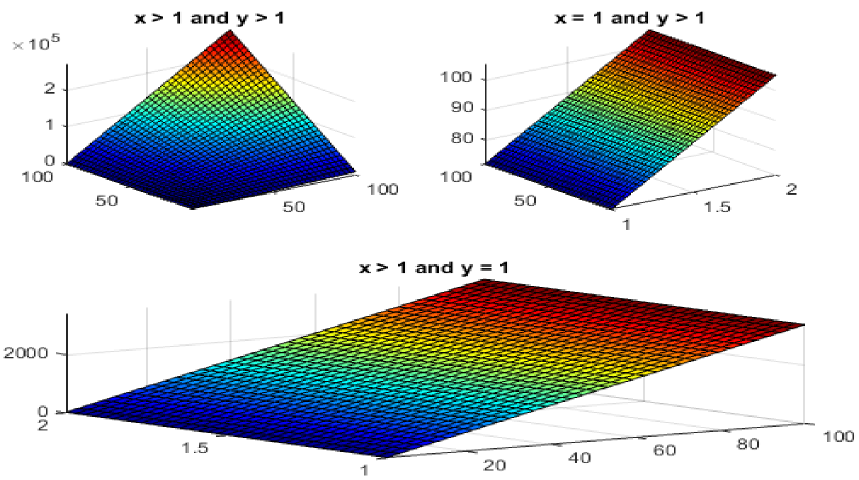


**Figure 5.** 3D Representation of $\Sigma\, SK_N^{\zeta}$.

Result 2.1: The product version of $SK_N^{\zeta}(G)$ *is*

$$\prod SK_N^{\zeta} = \begin{cases} 2^{12}3^{3}5 * 13^{2}\,(x-2)^{2}y(2y-4)17(x-2)(27xy-4y-4x+5) & if\ x>1, y>1 \\ 2^{7}3^{3}(26y-4)(7y-7) & if\ x=1, y>1 \\ 2^{10}3^{4}5^{2}13(x-2)^{2}(2x-5) & if\ x>1, y=1 \\ 24 & if\ x=1, y=1 \end{cases}$$

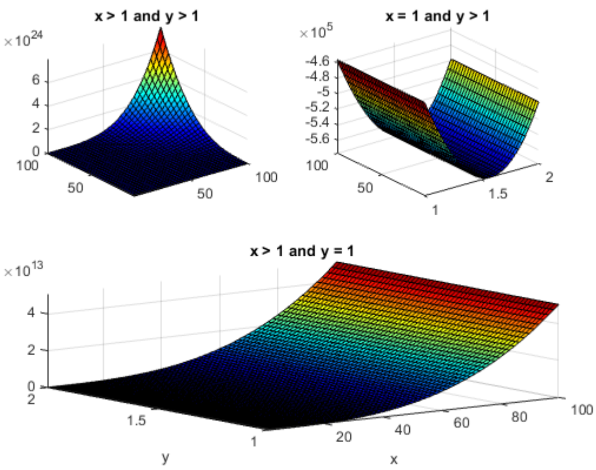


**Figure 6.** 3D Representation of $\Pi\, SK_N^{\zeta}$.

Theorem 2.2: The $SK1_N^{\zeta}$ index of graphene with x rows and y benzene rings is

$$SK1_N^{\zeta} = \begin{cases} \dfrac{309x + 290y + 3xy - 547}{2} & if\ x > 1, y > 1 \\ \dfrac{217y - 133}{2} & if\ x = 1, y > 1 \\ \dfrac{233x - 166}{2} & if\ x > 1, y = 1 \\ 48 & if\ x = 1, y = 1 \end{cases}$$

Proof: We establish the proof for the following four cases :

Case 1: We use the edge partition for *x > 1, y > 1* given in Table 1 in equation 2 and obtain,

$$SK1_N^{\zeta} = |'E_{(4,5)}| \left[\frac{20}{2}\right] + |'E_{(5,5)}| \left[\frac{25}{2}\right] + |'E_{(5,7)}| \left[\frac{35}{2}\right] + |'E_{(5,8)}| \left[\frac{40}{2}\right] + |'E_{(6,7)}| \left[\frac{42}{2}\right] + |'E_{(7,9)}| \left[\frac{63}{2}\right] + |'E_{(8,8)}| \left[\frac{64}{2}\right] + |'E_{(8,9)}| \left[\frac{72}{2}\right] + |'E_{(9,9)}| \left[\frac{81}{2}\right]$$

$$= 4\left[\frac{20}{2}\right] + x\left[\frac{25}{2}\right] + 8\left[\frac{35}{2}\right] + (2x - 4)\left[\frac{40}{2}\right] + (4y - 8)\left[\frac{42}{2}\right] + (2\ y)\left[\frac{63}{2}\right] + (x - 2)\left[\frac{64}{2}\right] + (2x - 4)\left[\frac{72}{2}\right] + (3xy - 4x - 4y + 5)\left[\frac{81}{2}\right]$$

$$= \frac{309x+290y+3xy-547}{2}.$$

Case 2: Using the edge partition for *x = 1, y > 1* given in Table 2 in equation 2 we obtain,

$$SK1_N^{\zeta} = |'E_{(4,4)}| \left[\frac{16}{2}\right] + |'E_{(4,5)}| \left[\frac{20}{2}\right] + |'E_{(5,7)}| \left[\frac{35}{2}\right] + |'E_{(6,7)}| \left[\frac{42}{2}\right] + |'E_{(7,7)}| \left[\frac{49}{2}\right]$$

$$= 2\left[\frac{16}{2}\right] + 4\left[\frac{20}{2}\right] + 4\left[\frac{35}{2}\right] + (4y - 8)\left[\frac{42}{2}\right] + (y - 1)\left[\frac{49}{2}\right]$$

$$= \frac{217y-133}{2}.$$

Case 3: Using the edge partition for *x > 1, y = 1* given in Table 3 in equation 2 we obtain,

$SK1_N^{\zeta}= \left|{}'E_{(4,4)}\right| \left[\frac{16}{2}\right] + \left|{}'E_{(4,5)}\right| \left[\frac{20}{2}\right] + \left|{}'E_{(5,5)}\right| \left[\frac{25}{2}\right] + \left|{}'E_{(5,7)}\right| \left[\frac{35}{2}\right] + \left|{}'E_{(5,8)}\right| \left[\frac{40}{2}\right] + \left|{}'E_{(7,8)}\right| \left[\frac{56}{2}\right] + \left|{}'E_{(8,8)}\right| \left[\frac{64}{2}\right] = 2 \left[\frac{16}{2}\right] + 4 \left[\frac{20}{2}\right] + (x - 2) \left[\frac{25}{2}\right] + 4 \left[\frac{35}{2}\right] + (2x - 4) \left[\frac{40}{2}\right] + 2 \left[\frac{56}{2}\right] + (2x - 5) \left[\frac{64}{2}\right]$

$$= \frac{233x-166}{2}.$$

Case 4: Using the edge partition for *x = 1*, *y=1*given in Table 4 in equation 2 we obtain,

$SK1_N^{\zeta}= \left|{}'E_{(4,4)}\right| \left[\frac{16}{2}\right] = 48.$

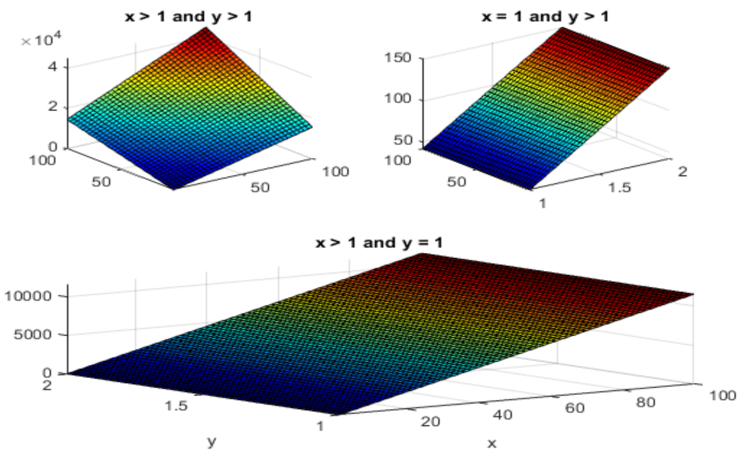


**Figure 7.** 3D Representation of $\sum SK1_N^{\zeta}$.

Result 2.2: The product version of $SK1_N^{\zeta}$(G) *is*

$$\prod SK1_N^{\zeta} = \begin{cases} 2^{14}3^5 5^5 7^3 xy\,(x-2)^3(4y-8)(3xy-4y-4x+5) & if\ x>1, y>1 \\ 2^7 3 * 5^2 7^4 (4y-8)(y-1) & if\ x=1, y>1 \\ 2^{17}5^5 7^2 (x-2)(2x-4)(2x-5) & if\ x>1, y=1 \\ 48 & if\ x=1, y=1 \end{cases}$$

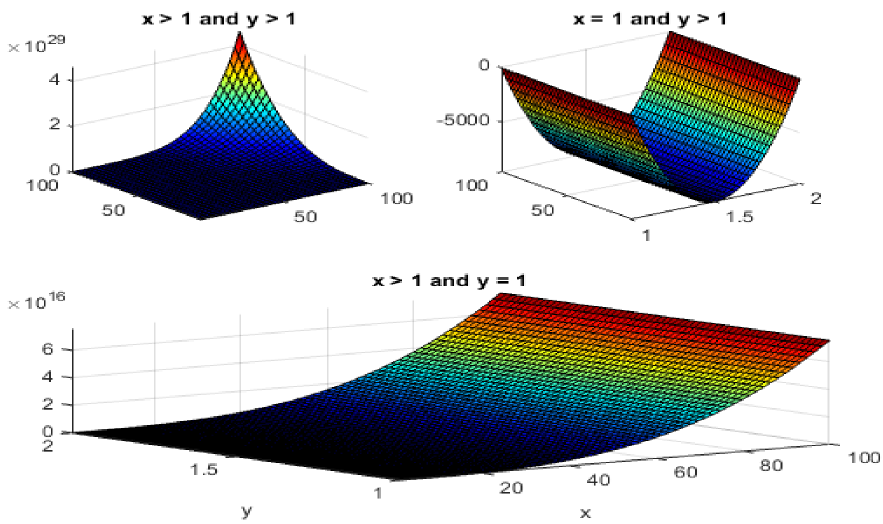


**Figure 8.** 3D Representation of $\prod SK1_N^{\zeta}$.

Theorem 2.3: The $SK2_N^{\zeta}$(G) index of Graphene with x rows and y benzene rings is

$$SK2_N^{\zeta} = \begin{cases} \dfrac{936xy - 660x - 871y + 846}{2} & if\ x > 1, y > 1 \\ 218y - 130 & if\ x = 1, y > 1 \\ \dfrac{475x - 339}{2} & if\ x > 1, y = 1 \\ 96 & if\ x = 1, y = 1 \end{cases}$$

Proof: We establish the proof for the following four cases :

Case 1: We use the edge partition for *x > 1, y > 1* given in Table 1 in equation 3 and obtain,

$$SK2_N^{\zeta} = |'E_{(4,5)}| \left[\frac{9}{2}\right]^2 + |'E_{(5,5)}| \left[\frac{10}{2}\right]^2 + |'E_{(5,7)}| \left[\frac{12}{2}\right]^2 + |'E_{(5,8)}| \left[\frac{13}{2}\right]^2 + |'E_{(6,7)}| \left[\frac{13}{2}\right]^2 + |'E_{(7,9)}| \left[\frac{16}{2}\right]^2 + |'E_{(8,8)}| \left[\frac{16}{2}\right]^2 + |'E_{(8,9)}| \left[\frac{17}{2}\right]^2 + |'E_{(9,9)}| \left[\frac{18}{2}\right]^2$$

$$= 4\left[\frac{9}{2}\right]^2 + x\left[\frac{10}{2}\right]^2 + 8\left[\frac{12}{2}\right]^2 + (2x-4)\left[\frac{13}{2}\right]^2 + (4y-8)\left[\frac{13}{2}\right]^2 + (2y)\left[\frac{16}{2}\right]^2 + (x-2)\left[\frac{16}{2}\right]^2 + (2x-4)\left[\frac{17}{2}\right]^2 + (3xy-4x-4y+5)\left[\frac{18}{2}\right]^2$$

$$= \frac{936xy - 660x - 871y + 846}{2}.$$

Case 2: Using the edge partition for *x = 1, y > 1* given in Table 2 in equation 3 we obtain,

$$SK2_N^{\zeta} = |'E_{(4,4)}| \left[\frac{8}{2}\right]^2 + |'E_{(4,5)}| \left[\frac{9}{2}\right]^2 + |'E_{(5,7)}| \left[\frac{12}{2}\right]^2 + |'E_{(6,7)}| \left[\frac{13}{2}\right]^2 + |'E_{(7,7)}| \left[\frac{14}{2}\right]^2$$

$$= 2\left[\frac{8}{2}\right]^2 + 4\left[\frac{9}{2}\right]^2 + 4\left[\frac{12}{2}\right]^2 + (4y-8)\left[\frac{13}{2}\right]^2 + (y-1)\left[\frac{14}{2}\right]^2$$

$$= 218y - 130.$$

Case 3: Using the edge partition for *x > 1, y = 1* given in Table 3 in equation 3 we obtain,

$$SK2_N^{\zeta} = |'E_{(4,4)}| \left[\frac{8}{2}\right]^2 + |'E_{(4,5)}| \left[\frac{9}{2}\right]^2 + |'E_{(5,5)}| \left[\frac{10}{2}\right]^2 + |'E_{(5,7)}| \left[\frac{12}{2}\right]^2 + |'E_{(5,8)}| \left[\frac{13}{2}\right]^2 + |'E_{(7,8)}| \left[\frac{15}{2}\right]^2 + ||'E_{(8,8)}| \left[\frac{16}{2}\right]^2$$

$$= 2\left[\frac{8}{2}\right]^2 + 4\left[\frac{9}{2}\right]^2 + (x-2)\left[\frac{10}{2}\right]^2 + 4\left[\frac{12}{2}\right]^2 + (2x-4)\left[\frac{13}{2}\right]^2 + 2\left[\frac{15}{2}\right]^2 + (2x-5)\left[\frac{16}{2}\right]^2$$

$$= \frac{475x - 339}{2}.$$

Case 4: Using the edge partition for *x = 1, y = 1* given in Table 4 in equation 3 we obtain,

$$SK2_N^{\zeta} = |'E_{(4,4)}| \left[\frac{8}{2}\right]^2 = 96.$$

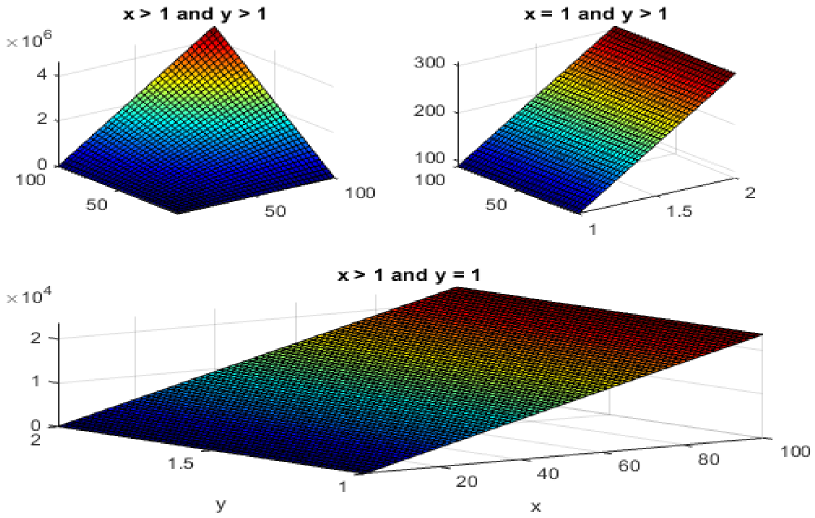


**Figure 9.** 3D Representation of $\Sigma\ SK2_N^\zeta$.

Result 2.3: The product version of $SK2_N^\zeta$(G) *is*

$$\prod SK2_N^\zeta = \begin{cases} 2^{16}3^{10}5^2 13^4 17^2 xy\,(x-2)^3(y-2)17(x-2)(3xy-4y-4x+5) & if\ x>1, y>1 \\ 2^9 3^6 13^2 (y-2)(49y-49) & if\ x=1, y>1 \\ 2^{13}3^8 5^4 13^2 (x-2)^2(2x-5) & if\ x>1, y=1 \\ 96 & if\ x=1, y=1 \end{cases}$$

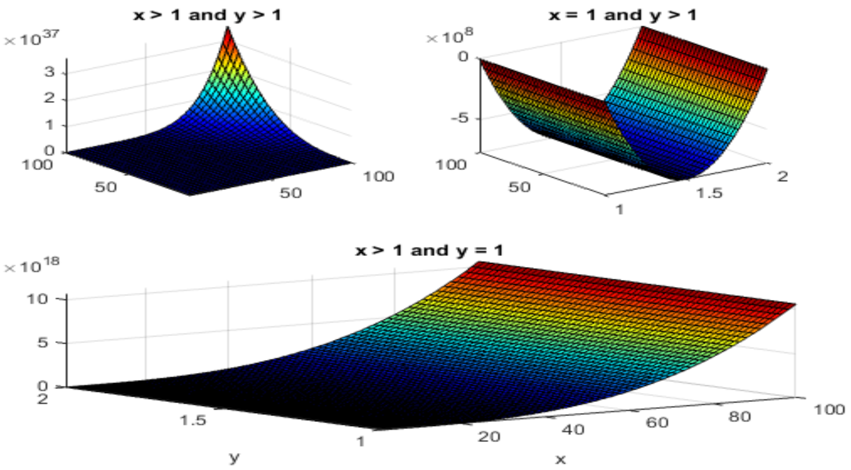


**Figure 10.** 3D Representation of $\prod SK2_N^\zeta$.

Theorem 2.4: The $mR_N^\zeta$(G) index of Graphene with x rows and y benzene rings is

$$mR_N^\zeta = \begin{cases} \dfrac{959x - 950y - 840xy + 266}{2520} & if\ x>1, y>1 \\ \dfrac{50y+41}{70} & if\ x=1, y>1 \\ \dfrac{196x+167}{280} & if\ x>1, y=1 \\ \dfrac{3}{2} & if\ x=1, y=1 \end{cases}$$

Proof: We establish the proof for the following four cases :

Case 1: We use the edge partition for *x > 1, y > 1* given in Table 1 in equation 4 and obtain,

$$mR_N^{\zeta} = |'E_{(4,5)}|\left[\frac{1}{max\{4,5\}}\right] + |'E_{(5,5)}|\left[\frac{1}{max\{5,5\}}\right] + |'E_{(5,7)}|\left[\frac{1}{max\{5,7\}}\right] + |'E_{(5,8)}|\left[\frac{1}{max\{5,8\}}\right] + |'E_{(6,7)}|\left[\frac{1}{max\{6,7\}}\right] + |'E_{(7,9)}|\left[\frac{1}{max\{7,9\}}\right] + |'E_{(8,8)}|\left[\frac{1}{max\{8,8\}}\right] + |'E_{(8,9)}|\left[\frac{1}{max\{8,9\}}\right] + |'E_{(9,9)}|\left[\frac{1}{max\{9,9\}}\right]$$

$$= \frac{959x-950y-840xy+266}{2520}.$$

Case 2: Using the edge partition for *x = 1, y > 1* given in Table 2 in equation 4 we obtain,

$$mR_N^{\zeta} = |'E_{(4,4)}|\left[\frac{1}{max\{4,4\}}\right] + |'E_{(4,5)}|\left[\frac{1}{max\{4,5\}}\right] + |'E_{(5,7)}|\left[\frac{1}{max\{5,7\}}\right] + |'E_{(6,7)}|\left[\frac{1}{max\{6,7\}}\right] + |'E_{(7,7)}|\left[\frac{1}{max\{7,7\}}\right]$$

$$= \frac{50y+41}{70}.$$

Case 3: Using the edge partition for *x > 1, y = 1* given in Table 3 in equation 4 we obtain,

$$mR_N^{\zeta} = |'E_{(4,4)}|\left[\frac{1}{max\{4,4\}}\right] + |'E_{(4,5)}|\left[\frac{1}{max\{4,5\}}\right] + |'E_{(5,5)}|\left[\frac{1}{max\{5,5\}}\right] + |'E_{(5,7)}|\left[\frac{1}{max\{5,7\}}\right] + |'E_{(5,8)}|\left[\frac{1}{max\{5,8\}}\right] + |'E_{(7,8)}|\left[\frac{1}{max\{7,8\}}\right] + |'E_{(8,8)}|\left[\frac{1}{max\{8,8\}}\right]$$

$$= \frac{196x+167}{280}.$$

Case 4: Using the edge partition for *x = 1, y = 1* given in Table 4 in equation 4 we obtain,

$$mR_N^{\zeta} = |'E_{(4,4)}|\left[\frac{1}{max\{4,4\}}\right]$$

$$= \frac{3}{2}.$$

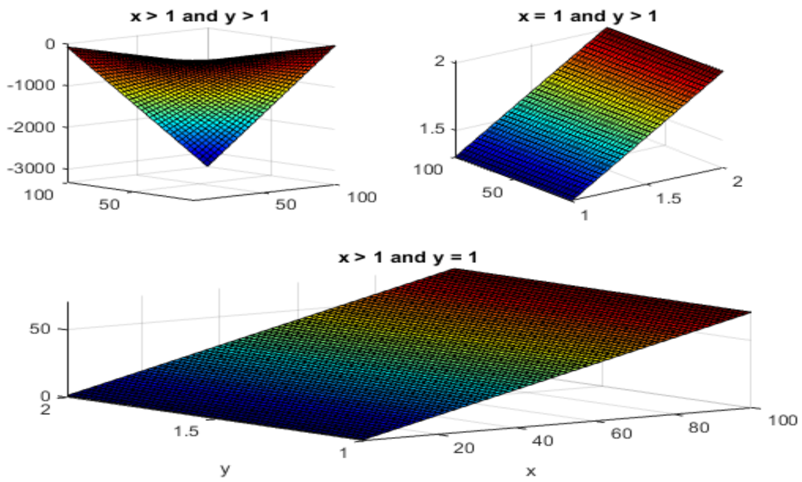


**Figure 11.** 3D Representation of $\Sigma\, mR_N^{\zeta}$.

Result 2.4: The product version of $mR_N^{\zeta}(G)$ *is*

$$\prod mR_N^{\zeta} = \begin{cases} \frac{xy(x-2)^3(y-2)(3xy-4y-4x+5)}{2^2 3^2 5^2 7^2} & if\ x>1, y>1 \\ \frac{2^5(y-1)(y-2)}{5*7^3} & if\ x=1, y>1 \\ \frac{(x-2)^2(2x-5)}{2^5 5^2 7} & if\ x>1, y=1 \\ \frac{3}{2} & if\ x=1, y=1 \end{cases}$$

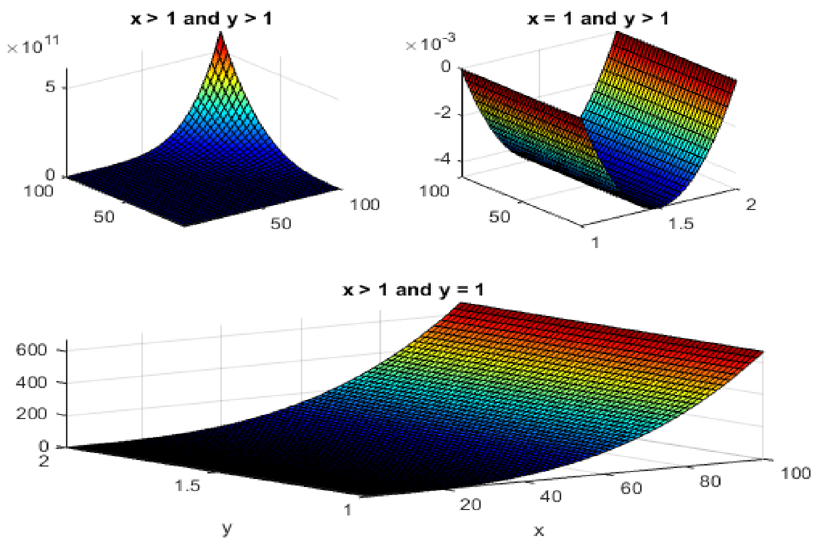


**Figure 12.** 3D Representation of $\prod mR_N^{\zeta}$.

Theorem 2.5 : The $ISI_N^{\zeta}$(G) index of graphene with x rows and y benzene rings is

$$ISI_N^{\zeta} = \begin{cases} \frac{49716x-44523y+214812xy-133228}{15912} & if\ x>1, y>1 \\ \frac{3843y-1121}{234} & if\ x=1, y>1 \\ \frac{19485x-6184}{1170} & if\ x>1, y=1 \\ 12 & if\ x=1, y=1 \end{cases}$$

Proof: We establish the proof for the following four cases:

Case 1: We use the edge partition for $x > 1, y > 1$ given in Table 1 in equation 5 and obtain,

$$ISI_N^{\zeta} = |E_{(4,5)}|\left[\frac{4*5}{4+5}\right] + |E_{(5,5)}|\left[\frac{5*5}{5+5}\right] + |E_{(5,7)}|\left[\frac{5*7}{5+7}\right] + |E_{(5,8)}|\left[\frac{5*8}{5+8}\right] + |E_{(6,7)}|\left[\frac{6*7}{6+7}\right] + |E_{(7,9)}|\left[\frac{7*9}{7+9}\right] + |E_{(8,8)}|\left[\frac{8*8}{8+8}\right] + |E_{(8,9)}|\left[\frac{8*9}{8+9}\right] + |E_{(9,9)}|\left[\frac{9*9}{9+9}\right]$$

$$= \left[\frac{80}{9}\right] + x\left[\frac{25}{10}\right] + \left[\frac{70}{3}\right] + (2x-4)\left[\frac{40}{13}\right] + (4y-8)\left[\frac{42}{13}\right] + \left[\frac{63y}{8}\right] + 4*(x-2) + (2x-4)\left[\frac{72}{17}\right] + (3xy-4x-4y+5)\left[\frac{9}{2}\right]$$

$$= \frac{49716x-44523y+214812xy-133228}{15912}.$$

Case 2: Using the edge partition for $x = 1, y > 1$ given in Table 2 in equation 5 we obtain,

$$ISI_N^{\zeta} = |E_{(4,4)}|\left[\frac{4*4}{4+4}\right] + |E_{(4,5)}|\left[\frac{4*5}{4+5}\right] + |E_{(5,7)}|\left[\frac{5*7}{5+7}\right] + |E_{(6,7)}|\left[\frac{6*7}{6+7}\right] + |E_{(7,7)}|\left[\frac{7*7}{7+7}\right]$$

$$= \frac{3843y-1121}{234}.$$

Case 3: Using the edge partition for $x > 1, y = 1$ given in Table 3 in equation 5 we obtain,

$$ISI_N^{\zeta} = |E_{(4,4)}|\left[\frac{4*4}{4+4}\right] + |E_{(4,5)}|\left[\frac{4*5}{4+5}\right] + |E_{(5,5)}|\left[\frac{5*5}{5+5}\right] + |E_{(5,7)}|\left[\frac{5*7}{5+7}\right] + |E_{(5,8)}|\left[\frac{5*8}{5+8}\right] + |E_{(7,8)}|\left[\frac{7*8}{7+8}\right] + |E_{(8,8)}|\left[\frac{8*8}{8+8}\right]$$

$$= \frac{19485x-6184}{1170}.$$

Case 4: Using the edge partition for $x = 1, y = 1$ given in Table 4 in equation 5 we obtain,

$$ISI_N^{\zeta} = |E_{(4,4)}|\left[\frac{4*4}{4+4}\right] = 12.$$

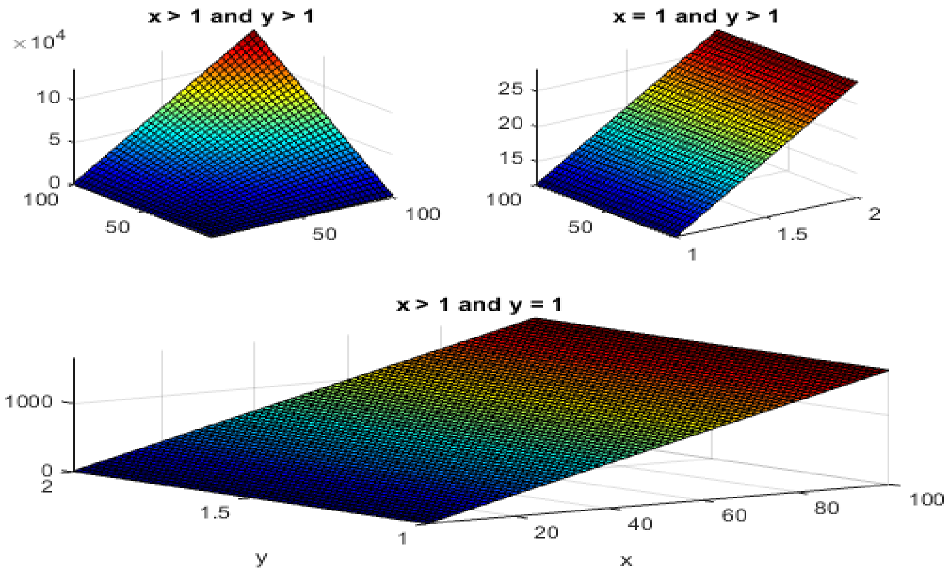


**Figure 13.** 3D Representation of $\Sigma\, ISI_N^{\zeta}$.

Result 2.4: The product version of $ISI_N^{\zeta}(G)$ is

$$\prod ISI_N^{\zeta} = \begin{cases} \dfrac{2^{13}3^4 5^4 7^3 xy(x-2)^3(y-2)(3xy-4y-4x+5)}{13^2 17} & if\ x>1, y>1 \\ \dfrac{2^8 5^2 7^3 (y-1)(y-2)}{3^2 13} & if\ x=1, y>1 \\ \dfrac{2^{15}5^3 7^2 (x-2)^2(2x-5)}{3^4 13} & if\ x>1, y=1 \\ 12 & if\ x=1, y=1 \end{cases}$$

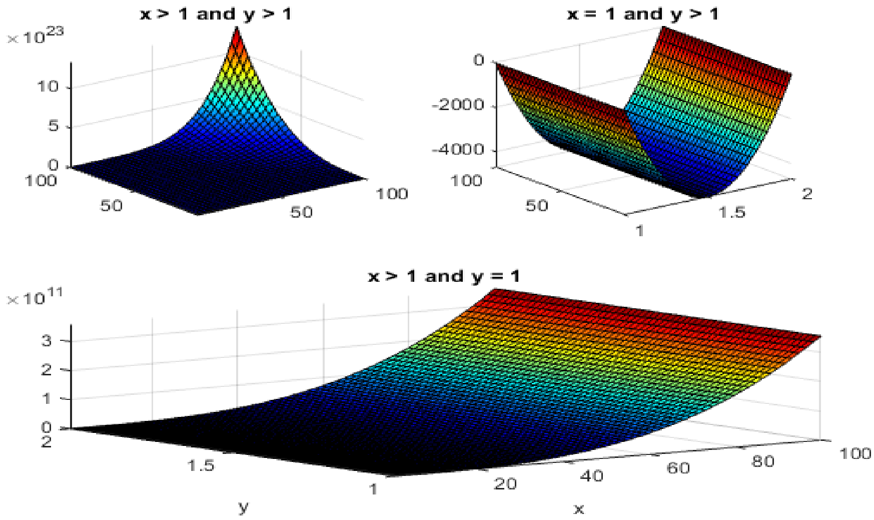


**Figure 14.** 3D Representation of $\prod ISI_N^{\zeta}$.

## 4. Conclusions

The computation of various topological indices of graphs associated with chemical graphs enables the analysis of molecules and study of how the indices relate to the molecular properties. We estimated a few topological indices based on the neighborhood degree and obtained results based on both the sum and products of the cardinality of edge partitions corresponding to 4 different Graphene structures. We also presented the 3D representations (Figures 5 – 14) of these indices using MATLAB. We envisage applying these definitions to the line graph, subdivision graphs, and total graphs of the Graphene structure in future work. Further, we would establish the relationship between these indices and some chemical properties of graphene.

### Funding

This research received no external funding.

### Acknowledgments

This research has no acknowledgment.

### Conflicts of Interest

The authors declare no conflict of interest.

## References

1. Aslam, A.; Guirao, J.; Ahmad, S.; Gao, W. Topological Indices of the Line Graph of Subdivision Graph of Complete Bipartite Graphs. *Applied Mathematics & Information Sciences* **2017**, *11*, 1631-1636, http://dx.doi.org/10.18576/amis/110610.
2. Ahmad, M.; Afzal, D.; Nazeer, W.; Kang, S. On topological indices of octagonal network. *Far East Journal of Mathematical Sciences* **2017**, *102*, 2563-2571, http://dx.doi.org/10.17654/MS102112563.
3. Deutsch, E.; Klavžar, S. M-polynomial and Degree-based Topological Indices. *Iranian Journal of Mathematical Chemistry* **2015**, *6*, 93-102, https://dx.doi.org/10.22052/ijmc.2015.10106.
4. The many faces of nanotech. *Nature Nanotechnology* **2007**, *2*, 585-585, https://doi.org/10.1038/nnano.2007.308.
5. Gutman, I. Molecular graphs with minimal and maximal Randic indices. *Croatica Chemica Acta* **2002**, *75*, 357-369.

6. Gutman, I. Degree-Based Topological Indices. *Croatica Chemica Acta* **2013**, *86*, 351-361, http://dx.doi.org/10.5562/cca2294.
7. Farrukh, F.; Hafi, S.; Farooq, R.; Farahani, M. Calculating some topological indices of SiO2 layer structure [252]. *Journal of Informatics and Mathematical Sciences* **2016**, *8*, 181-187, http://dx.doi.org/10.26713%2Fjims.v8i3.445.
8. West, D.B. *An Introduction To Graph Theory*. Prentice hall, Inc. New Jersey, **1996**.
9. Sedlar, J.; Stevanović, D.; Vasilyev, A. On the inverse sum indeg index. *Discrete Applied Mathematics* **2015**, *184*, 202-212, https://doi.org/10.1016/j.dam.2014.11.013.
10. Sridhara, G.; Rajesh Kanna, M.R.; Indumathi, R.S. Computation of Topological Indices of Graphene. *Journal of Nanomaterials* **2015**, *2015*, https://doi.org/10.1155/2015/969348.
11. Jagadeesh, R.; Rajesh Kanna, M.R.; Indumathi, R.S. Some results on topological indices of graphene. *Nanomaterials and Nanotechnology* **2016**, *6*, 1–6, https://doi.org/10.1177%2F1847980416679626.
12. Rachanna, R.K.; Vijayalaxmi, S.; Shigehalli. Computing Some Degree-Based Topological Indices of Graphene. *Indonesian Journal of Electrical Engineering and Informatics* **2017**, *5*, 115-161, http://dx.doi.org/10.11591/ijeei.v5i2.258.
13. Akhter, S.; Imran, M.; Gao, W.; Farahani, M. On topological indices of honeycomb networks and Graphene networks [253]. *Hacettepe Journal of Mathematics and Statistics* **2018**, *47*, 19–35.
14. Kwun, Y.; Ahmad, J.; Nazeer, W.; Khalid, W.; Kang, S. Topological Invariants Of Molecular Graph Of Graphene. *JP Journal of Geometry and Topology* **2018**, *21*, 95-103, http://dx.doi.org/10.17654/GT021020095.
15. Shigehalli, V.S.; Kanabur, R. Computation of New Degree-Based Topological Indices of Graphene. *Journal of Mathematics* **2016**, *2016*, https://doi.org/10.1155/2016/4341919.
16. Mondal, S.; De, N.; Pal, A. Topological properties of Graphene using some novel neighborhood degree-based topological indices. *International Journal of Mathematics for Industry* **2019**, *11*, https://dx.doi.org/10.1142/S2661335219500060.
17. Berhe, M.; Wang, C. Computation of certain topological coindices of graphene sheet and C4C8(S) nanotubes and nanotorus. *Applied Mathematics and Nonlinear Sciences* **2019**, *4*, 455-468, https://doi.org/10.2478/AMNS.2019.2.00043.
18. Parashivamurthy, H.L.; Kanna M R, R.; Jagadeesh, R. Some Topological Indices and their Polynomials of Graphene. *Oriental Journal Of Chemistry* **2019**, *35*, 1514-1518, http://dx.doi.org/10.13005/ojc/350506.
19. Sudhakara, K.; Guruprasad, P.S.; Sriraj, M.A. Some edge degree based topological indices of Graphene. *Proceedings of the Jangjeon Mathematical Society* **2020**, *23*, 253-270.
20. Zhu, Y.; Murali, S.; Cai, W.; Li, X.; Suk, J.W.; Potts, J.R.; Ruoff, R.S. Graphene and Graphene Oxide: Synthesis, Properties, and Applications. *Advanced Materials* **2010**, *22*, 3906-3924, https://doi.org/10.1002/adma.201001068.
21. Huang, X.; Qi, X.; Boey, F.; Zhang, H. Graphene-based composites. *Chemical Society Reviews* **2012**, *41*, 666-686, https://doi.org/10.1039/c1cs15078b.
22. Liu, D.-X.; Li, X.-F.; Zhang, X.-H.; Cao, X.; Zhu, X.-J.; Shi, D. Interface Magnetism in Topological Armchair/Cove-Edged Graphene Nanoribbons. *The Journal of Physical Chemistry C* **2020**, *124*, 15448-15453, https://doi.org/10.1021/acs.jpcc.0c04152.
23. Rada, J. Vertex-Degree Based Topological Indices of Graphene. *Polycyclic Aromatic Compounds* **2020**, 1-9, https://doi.org/10.1080/10406638.2020.1785897.
24. Kwun, Y.C.; Virk, A.U.R.; Rafaqat, M.; Rehman, M.U.; Nazeer, W. Some reversed degree-based topological indices for graphene. *Journal of Discrete Mathematical Sciences and Cryptography* **2019**, *22*, 1305-1314, https://doi.org/10.1080/09720529.2019.1691329.
25. Ahmad, A. Computation of certain topological properties of para-line graph of honeycomb networks and graphene. *Discrete Mathematics, Algorithms and Applications* **2017**, *09*, https://doi.org/10.1142/S1793830917500641.
26. Arockiaraj, M.; Clement, J.; Tratnik, N.; Mushtaq, S.; Balasubramanian, K. Weighted Mostar indices as measures of molecular peripheral shapes with applications to graphene, graphyne and graphdiyne nanoribbons. *SAR and QSAR in Environmental Research* **2020**, *31*, 187-208, https://doi.org/10.1080/1062936X.2019.1708459.
27. Putz, M.V.; Ori, O. Topological Symmetry Transition between Toroidal and Klein Bottle Graphenic Systems. *Symmetry* **2020,** *12*, https://doi.org/10.3390/sym12081233.
28. Anwar Saleh.; Sophia Shalini, G. B.; Dhananjayamurthy, B. V. The Reduced Neighborhood Topological Indices and RNM − Polynomial for the Treatment of COVID-19. *Biointerface Research in Applied Chemistry* **2021**, 11(4), 11817 - 11832, https://doi.org/10.33263/BRIAC114.1181711832
29. Mondal, S.; De, N.; Siddiqui, M. K..; Pal, A. Topological Properties of Para-Line Graph of Some Convex Polytopes Using Neighborhood M-Polynomial. *Biointerface Research in Applied Chemistry* **2021**, 11(3), 9915 - 9927, https://doi.org/10.33263/BRIAC113.99159927
30. Mondal, S.; De, N.; Pal, A. On some new neighbourhood degree based indices. Acta Chemica Iasi 2019, 27, 31-46, https://doi.org/10.2478/achi-2019-0003.

31. Mondal, S.; De, N.; Pal, A. QSPR analysis of some novel neighborhood degree based topological descriptors. arXiv:1906.066602019.
32. Asif, F.; Zahid, Z.; Zafar, S.; Farahani, M.R.; Gao, W. On topological properties of some convex polytopes by using line operator on their subdivisions. *Hacet. J. Math. Stat*. **2019**, 49, 1-10, https://doi.org/10.15672/HJMS.2019.671.
33. Foruzanfar, Z.; Asif, F.; Zahid, Z.; Zafar, S.; Farahani, M.R. $ABC4$ and $GA5$ indices of para-line graph of some convex polytopes. *Stat., Optim. Inf. Comput*. **2019**, 7, 192-197, https://doi.org/10.19139/soic.v7i1.346.
34. Liu, J.B.; Zhao, J.; He, H.; Shao, Z. Valency-Based Topological Descriptors and Structural Property of the Generalized Sierpinski Networks. *J. Stat. Phys*. **2019**, 177, 1131-1147, https://doi.org/10.1007/s10955-019-02412-2.
35. Mondal, S.; De, N.; Pal, A. Topological properties of Graphene using some novelneighborhood degree-based topological indices. *Int. J. Ind. Math*. **2020**, 11, https://doi.org/10.1142/S2661335219500060.