A study on the M-Polynomials and Degree based Topological Indices of Graphene

Abstract

The exceptional properties of graphene have sparked intense research interest, necessitating a deeper understanding of its molecular architecture and chemical behavior. Degree-based topological indices are mathematical descriptors used in theoretical chemistry and materials science to quantify the structural properties of molecules and materials. This study explores the application of some degree-based topological indices and the M-polynomial to unravel graphene's chemical properties. Our investigation of some novel topological indices, offers unique insights into the structure-property relationships governing graphene's behavior. These findings highlight the versatility of degree-based topological methods in advancing materials science research and facilitating the development of graphene-based technologies. By harnessing the power of mathematical modeling, this work will help future material design and engineering initiatives.

Keywords: Topological indices, Chemical Graph Theory, M-Polynomial

2020 Mathematics Subject Classification: 05C90; 05C92

1 Introduction

Chemical Graph Theory is an interdisciplinary field in which the molecular structure of a chemical compound is analyzed as a mathematical graph, and related mathematical questions are investigated through graph theoretical and computational techniques. One of the most important ideas employed in Chemical Graph Theory is the so called chemical indices, also known as topological indices. Topological indices are numerical values associated with the graph structure of a chemical compound. For this reason, topological indices are generally considered as descriptors of chemical structures. Topological indices include distance based indices, degree based indices and spectral based indices

(1; 2). They play important role in Quantitative Structure Activity Relationship (QSAR) and Quantitative Structure Property Relationship (QSPR) (1; 11; 12). Many degree based topological indices which correspond to chemical properties of the material under an investigation are generated by M-polynomials.

A graph G is an ordered triple (V(G),E(G),Ψ_G) consisting of a nonempty set V(G) of vertices, a set E(G) of edges, disjoint from V(G) and an incident function Ψ_G which associates to each edge of G, an unordered pair, not necessarily distinct, of vertices of G. If no confusion arises, we write V, E, and Ψ respectively instead of V(G), E(G) and Ψ_G (14).

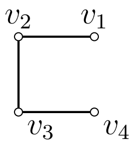


Fig. 1. M-polynomials

If an edge e joins two vertices u & v of G, we say that u & v are adjacent and also e is incident with u and v. In this case we write either uv $\in$ E or u$\sim$v. The number of edges incident with a vertex u of a graph G is denoted by d_G(u) or simply d(u) (14). In Fig. 1, v_1 and v_2 are adjacent while v_1 and v_3 are not.

Graphene is a material extracted from graphite and is made up of pure carbon, one of the most important elements in nature and which we find in daily objects like the lead of a pencil. It is the world's thinnest, strongest and most electrical and thermal conductive material. Graphene stands out for being tough, flexible, light and with a high resistance. It is calculated that this material is 200 times more resistant than steel and five times lighter than aluminium. It has numerous applications from sensors to batteries to nanotubes.Carbon fibres are very important in the constrution of aeroplanes.

2 Basic Definitions

Let $G = (V, E)$ be a graph. For $i, j \geq 1$, let $m_{i,j}$ denote the number of edges $e = uv \in E(G)$ such that $\{d_u(G), d_v(G)\} = \{i, j\}$, where $d_u(G)$ is the degree of vertex u in G.

The *M-polynomial* of G (10)is defined as

$$M(G; x, y) = \sum_{i \leq j} m_{i,j} x^i y^j$$

The M-polynomial encodes information about edge-degree distributions in G. Also It is useful for computing various degree-based topological indices of chemical graphs. We list some well known topological indices below.

1. In 1975, Milan Randic introduced the Randic Index (2), denoted by R(G) as R(G) = $\sum_{uv \in G} \frac{1}{\sqrt{d_u d_v}}$
2. Trinajstic et al. in 1972 defined the first and secong Zagreb indices(1) as follows: First Zagreb Index, M_1(G) = $\sum_{uv \in G}(d_u + d_v)$Second Zagreb Index, M_2(G) = $\sum_{uv \in G}(d_u.d_v)$
3. In 2010, Furtula et al. defined the Augmented Zagreb Index (1) as AZI(G) = $\sum_{u \sim v} \left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3$
4. Vukičević et al. in 2009 defined the Geometric Arithmetic Index (1) by GA(G) = $\sum_{uv \in E} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)}$

5. In 2012, Zhong defined the Harmonic Index (1) H(G) as H(G) = $\sum_{u\sim v} \frac{2}{d_u + d_v}$
6. The Atom - Bond Connectivity Index was defined by Estrada et al. in 1998 (1) as ABC(G) = $\sum_{u\sim v} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$

In this article, we used edge partitiion approach, where the edges of a graphene structure are divided into various groups according to the degrees of the end vertices of edges.

We begin with two hexagons joined each other at an edge (Cf Fig. 2). This is taken as a single unit of graphene.

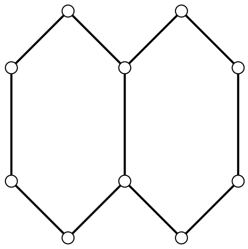


Fig.2 one unit of graphene

The process is continued to form an (m, n) chain (m rows & n columns) of each unit of graphene (Cf Fig. 3). Let us call this a graphene with dimension mn.

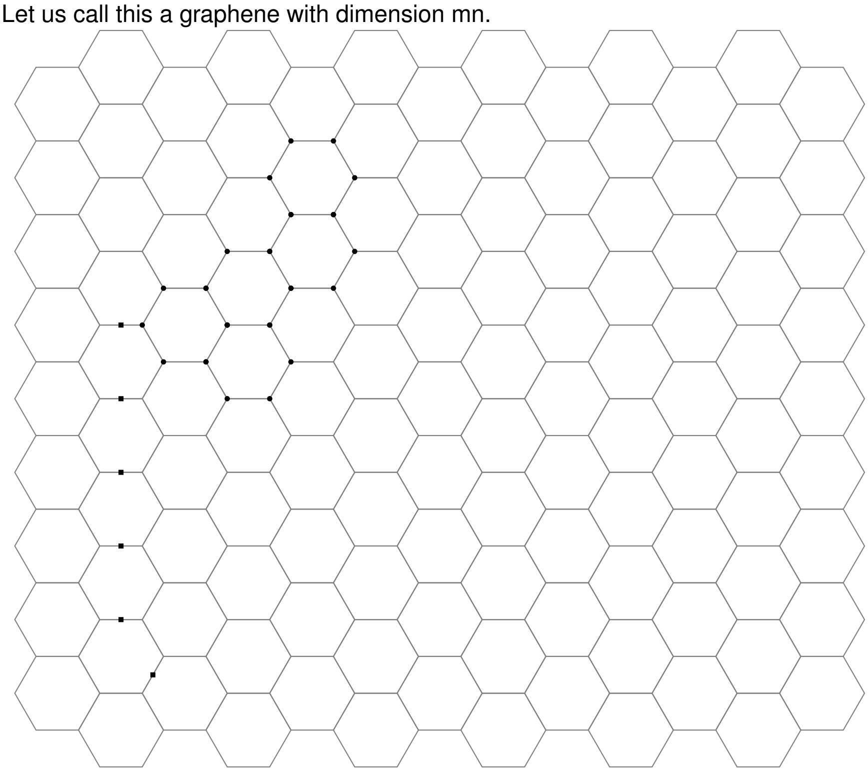


Fig. 3 an (m, n) chain of graphene structure

List 1 : The edges are partitioned into (2, 2), (2,3) & (3,3) groups as follows.

Edge Partition	(2, 2)	(2, 3)	(3, 3)
m= 1	6	8n - 4	2n - 1
m $>$ 1	m + 4	2m + 8n - 4	6mn - 4n - m - 1

In all the discussions below we assume G to be an (m, n) chain of graphene.

3 M-polynomial of an (m, n) chain of graphene

The M-polynomial of an (m, n) chain of Graphene G is given by

$$M(G,m,n) = \begin{cases} 6x^2y^2 + (8n-4)x^2y^3 + (2n-1)x^3y^3 & \text{for } m = 1, \\ (m+4)x^2y^2 + (2m+8n-4)x^2y^3 + (6mn-4n-m-1)x^3y^3 & \text{for } m > 1. \end{cases}$$

4 Main Results

Result 1. Let G be an (m, n) graphene. Then the Randic Index,

$$R(G) = \begin{cases} \dfrac{(24+2\sqrt{6})n + 8\sqrt{6} - 12}{3\sqrt{6}} & \text{if } m = 1, \\ \dfrac{m+4}{2} + \dfrac{2m+8n-4}{\sqrt{6}} + \dfrac{6mn-4n-mn-1}{3} & \text{if } m > 1. \end{cases}$$

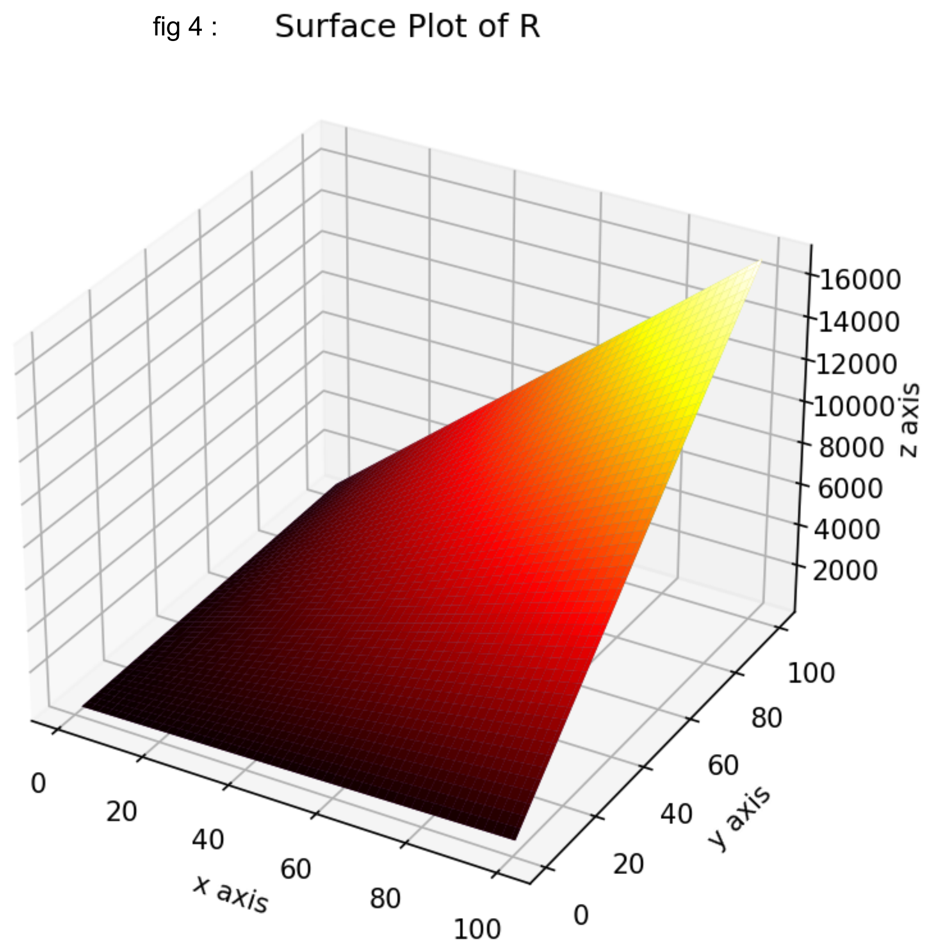
Proof. R(G) = $\sum_{uv\in E} \dfrac{1}{\sqrt{d_u d_v}}$
When m = 1

$$\begin{aligned} R &= 6.\frac{1}{\sqrt{2.2}} + 8n - 4\frac{1}{\sqrt{2.3}} + (2n-1)\frac{1}{\sqrt{3.3}} \\ &= 3 + \frac{8n-4}{\sqrt{6}} + \frac{2n-1}{3} \\ &= \frac{9\sqrt{6} + 3(8n-4) + (2n-1)\sqrt{6}}{3\sqrt{6}} \\ &= \frac{(24+2\sqrt{6})n + 8\sqrt{6} - 12}{3\sqrt{6}} \end{aligned}$$

When m $>$ 1

$$\begin{aligned} R &= (m+4)\frac{1}{\sqrt{2.2}} + (2m+8n-4)\frac{1}{\sqrt{2.3}} + \frac{(6mn-4n-m-1)}{\sqrt{3.3}} \\ &= \frac{m+4}{2} + \frac{2m+8n-4}{\sqrt{6}} + \frac{6mn-4n-mn-1}{3} \end{aligned}$$

fig 4 : Surface Plot of R



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Result 2. The first Zagreb Index of G,

$$M_1 = \begin{cases} 26(2n-1) & \text{for } m = 1, \\ 8m + 16n + 36mn - 10 & \text{for } m > 1. \end{cases}$$

Proof. $M_1 = \sum(d_u + d_v)$
When m = 1

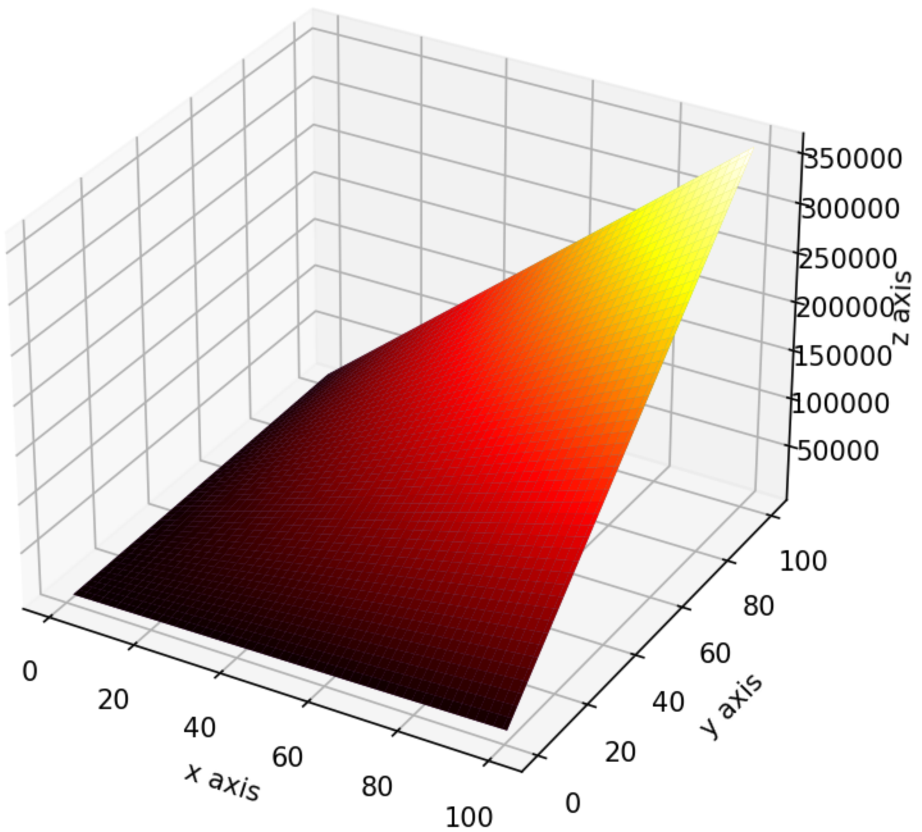
$$\begin{aligned} M_1 &= 6(2+2) + (8n-4)(2+3) + (2n-1)(3+3) \\ &= 24 + 40m - 20 + 12n - 6 \\ &= 52n - 26 \\ &= 26(2n-1) \end{aligned}$$

When m $>$ 1

$$\begin{aligned} M_1 &= (m+4)(2+2) + (2m+8n-4)(2+3) + (6mn-4n-m-1)(3+3) \\ &= 4m + 16 + 10m + 40n - 20 + 36mn - 24n - 6m - 6 \\ &= 8m + 16n + 36mn - 10 \end{aligned}$$

□

fig 5 : Surface Plot of M1



Result 3. The second Zagreb Index of G,

$$M_2 = \begin{cases} 66n - 9 & \text{if } m = 1, \\ 7m + 12n + 54mn - 17 & \text{if } m > 1. \end{cases}$$

Proof. $M_2 = \sum(d_u.d_v)$
When m = 1

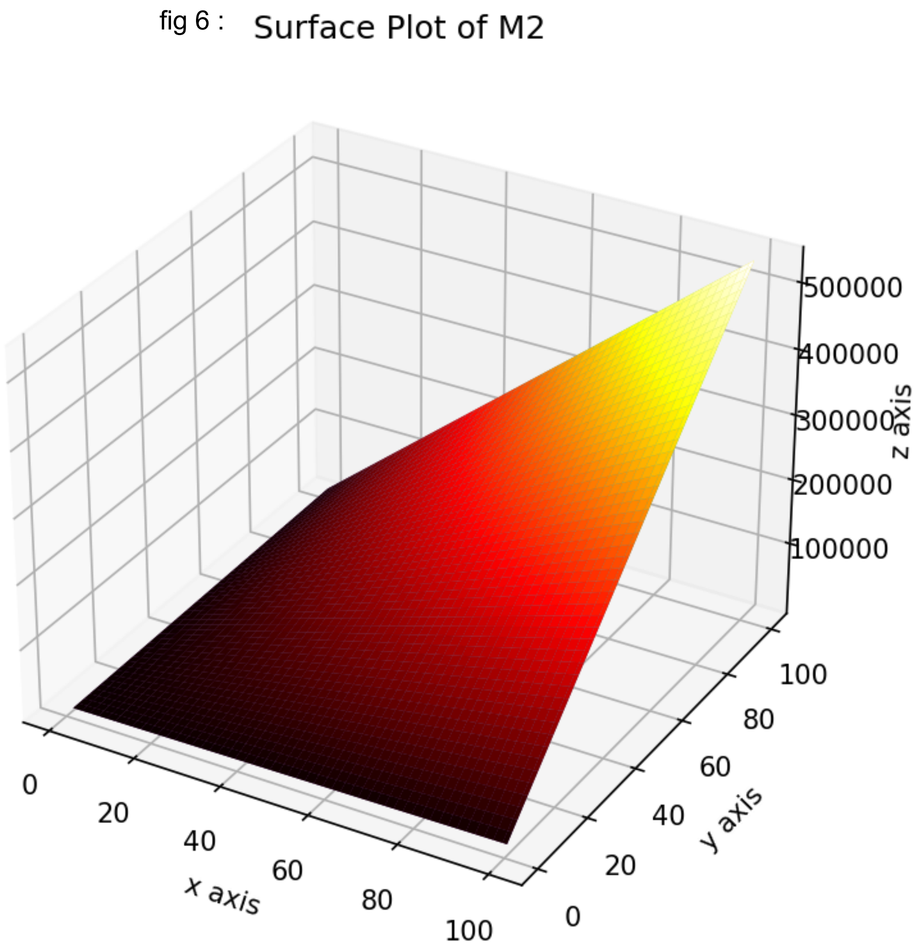
$$\begin{aligned} M_1 &= 6(2.2) + (8n-4)(2.3) + (2n-1)(3.3) \\ &= 24 + 48n - 24 + 18n - 9 \\ &= 66n - 9 \end{aligned}$$

When m $>$ 1

$$\begin{aligned} M_1 &= (m+4)(2.2) + (2m+8n-4)(2.3) + (6mn-4n-m-1)(3.3) \\ &= 4m + 16 + 12m + 48n - 24 + 50mn - 36n - 9m - 9 \\ &= 7m + 12n + 54mn - 17 \end{aligned}$$

□

fig 6 :



Result 4. The Augmented Zagreb Index of G is

$$AZI(G) = \begin{cases} \frac{82n+7}{4} & \text{if } m = 1, \\ \frac{15}{4}m + 7n + \frac{27}{2}mn - \frac{41}{4} & \text{if } m > 1. \end{cases}$$

Proof. AZI(G) = $\sum \left[\frac{d_u d_v}{d_u + d_v - 2}\right]^3$
When m = 1,

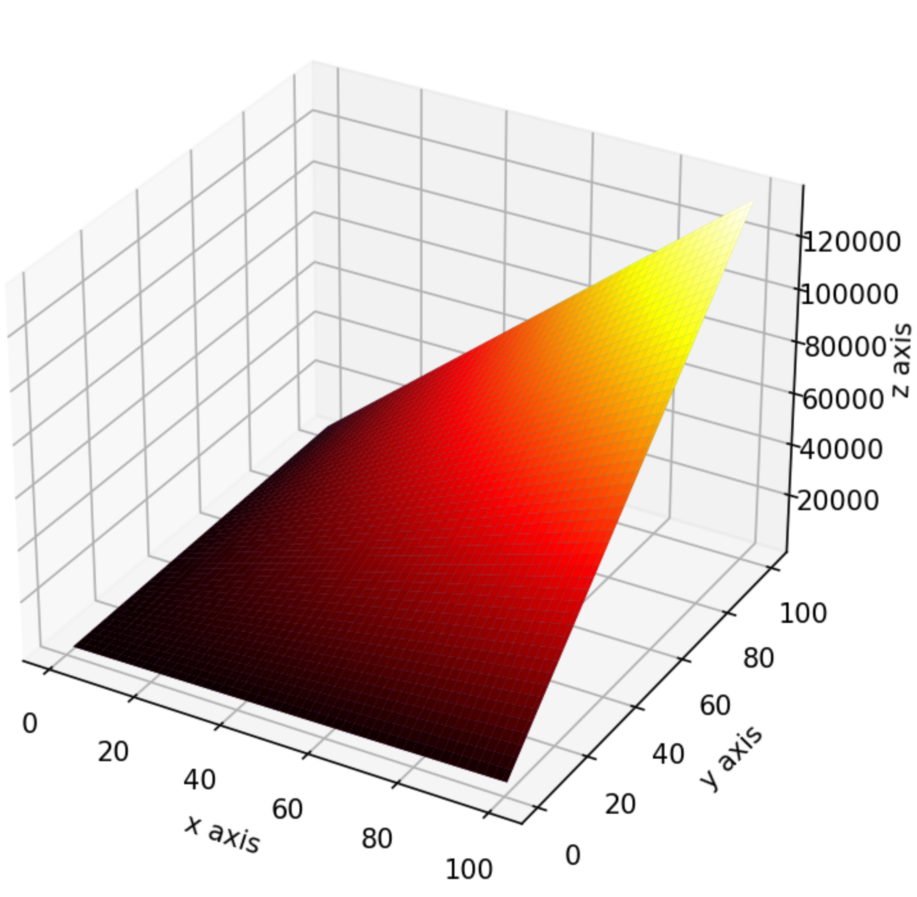
$$AZI = 6\left[\frac{2.2}{2+2-2}\right]^3 + (8n-4)\left[\frac{2.3}{2+3-2}\right]^3 + (2n-1)\left[\frac{3.3}{3+3-2}\right]^3$$
$$= \frac{82n+7}{4}$$

When m > 1,

$$AZI = (m+4)\left[\frac{2.2}{2+2-2}\right]^3 + (2m+8n-4)\left[\frac{2.3}{2+3-2}\right]^3 + (6mn-4n-m-1)\left[\frac{3.3}{3+3-2}\right]^3$$
$$= \frac{15}{4}m + 7n + \frac{27}{2}mn - \frac{41}{4}$$

□

fig 7 : Surface Plot of AZI



Result 5. The Geometric Arithmetic Index of G is

$$GA(G) = \begin{cases} \frac{1}{5}\left[(16\sqrt{6}+10)n + (25-8\sqrt{6})\right] & \text{if } m = 1, \\ \frac{4\sqrt{6}}{5}m + \frac{16\sqrt{6}-20}{5}n + 6mn + 3 & \text{if } m > 1. \end{cases}$$

Proof. GA(G) = $\sum_{uv \in E} \frac{\sqrt{d_u d_v}}{\frac{1}{2}(d_u + d_v)}$

When m = 1,

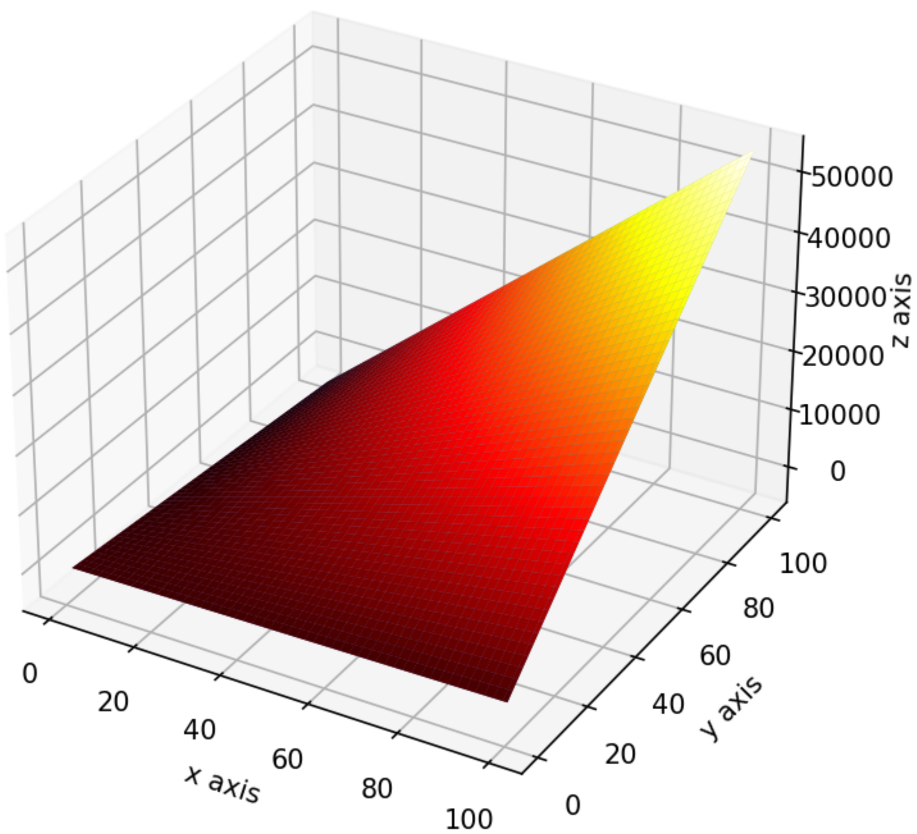
$$
\begin{aligned}
GA &= 6\frac{2\sqrt{4}}{4} + (8n-4)\frac{2\sqrt{6}}{5} + (2n-1)\frac{2\sqrt{9}}{6} \\
&= 6 + \frac{2\sqrt{6}}{5}8n - 4\frac{2\sqrt{6}}{5} + (2n-1) \\
&= \frac{1}{5}\left[(16\sqrt{6}+10)n + (25-8\sqrt{6})\right]
\end{aligned}
$$

When m $>$ 1,

$$
\begin{aligned}
GA &= (m+4) + (2m+8n-4)\frac{2\sqrt{6}}{5} + (6mn-4n-m-1) \\
&= (m+4) + \frac{4\sqrt{6}}{5}m + \frac{16\sqrt{6}}{5}n - \frac{8\sqrt{6}}{5} + 6mn - 4n - m - 1 \\
&= \frac{4\sqrt{6}}{5}m + \frac{16\sqrt{6}-20}{5} + 6mn + 3
\end{aligned}
$$

□

fig 8 : Surface Plot of GA



Result 6. The Harmonic Index of G is

$$H(G) = \begin{cases} \frac{58n+16}{15} & \text{if } m = 1, \\ \frac{29m+56n+60mn+2}{30} & \text{if } m > 1. \end{cases}$$

Proof. H(G) = $\sum \frac{2}{d_u + d_v}$
When m = 1,

$$\begin{aligned} H &= 6\frac{2}{2+2} + (8n-4)\frac{2}{2+3} + (2n-1)\frac{2}{3+3} \\ &= \frac{6}{2} + \frac{16n-8}{5} + \frac{(2n-1)}{3} \\ &= \frac{90+96n-48+20n-10}{30} \\ &= \frac{116n+32}{30} \\ &= \frac{58n+16}{15} \end{aligned}$$

When m $>$ 1,

$$\begin{aligned} H &= \frac{(m+4)}{2} + \frac{2}{5}(2m+8n-4) + \frac{1}{3}(6mn-4n-m-1) \\ &= \frac{(m+4)}{2} + \frac{4m+16n-8}{5}m + \frac{6mn-4n-m-1}{3} \\ &= \frac{15m+60+24m+96n-48+60mn-40n-10m-10}{30} \\ &= \frac{29m+56n+60mn+2}{30} \end{aligned}$$

□

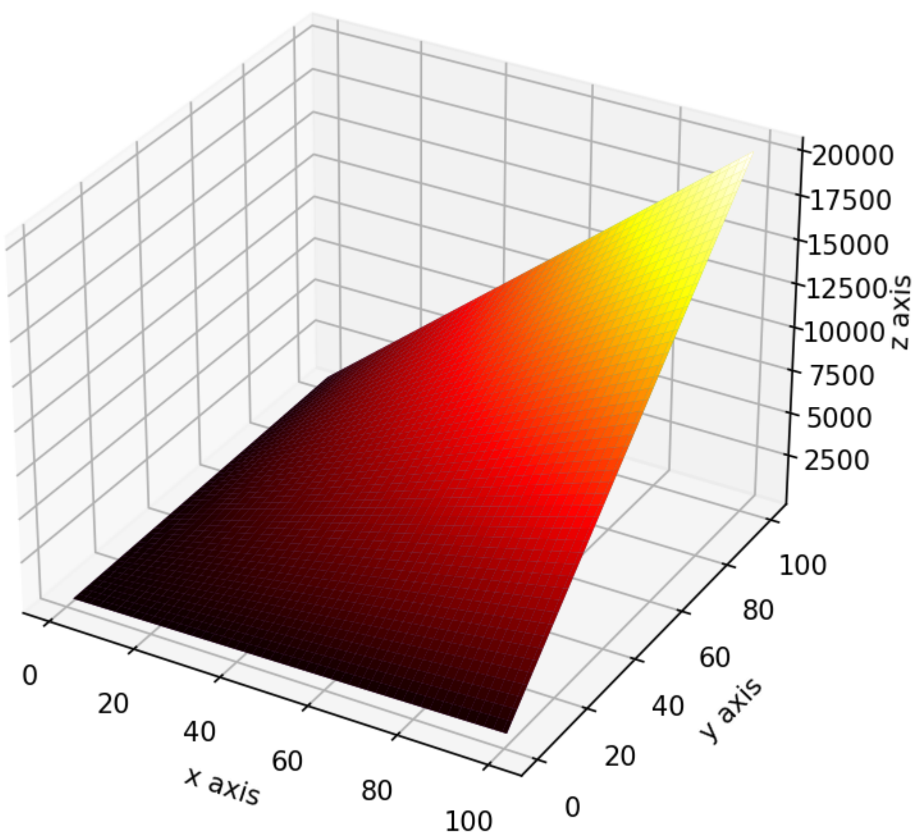


fig 9 : Surface Plot of H

Result 7. The Sum Connectivity Index of G is

$$SCI(G) = \begin{cases} \dfrac{(8\sqrt{6}+2\sqrt{5})n-(4\sqrt{6}+\sqrt{5})}{\sqrt{30}}+3 & \text{if } m=1, \\ \dfrac{(\sqrt{30}+4\sqrt{6}-2\sqrt{5})m+(16\sqrt{6}-8\sqrt{5})n+12\sqrt{5}mn+(4\sqrt{30}\,8\sqrt{6}-2\sqrt{5})}{2\sqrt{30}} & \text{if } m>1. \end{cases}$$

Proof. SCI(G) = $\sum \dfrac{1}{\sqrt{d_u+d_v}}$

When m = 1,

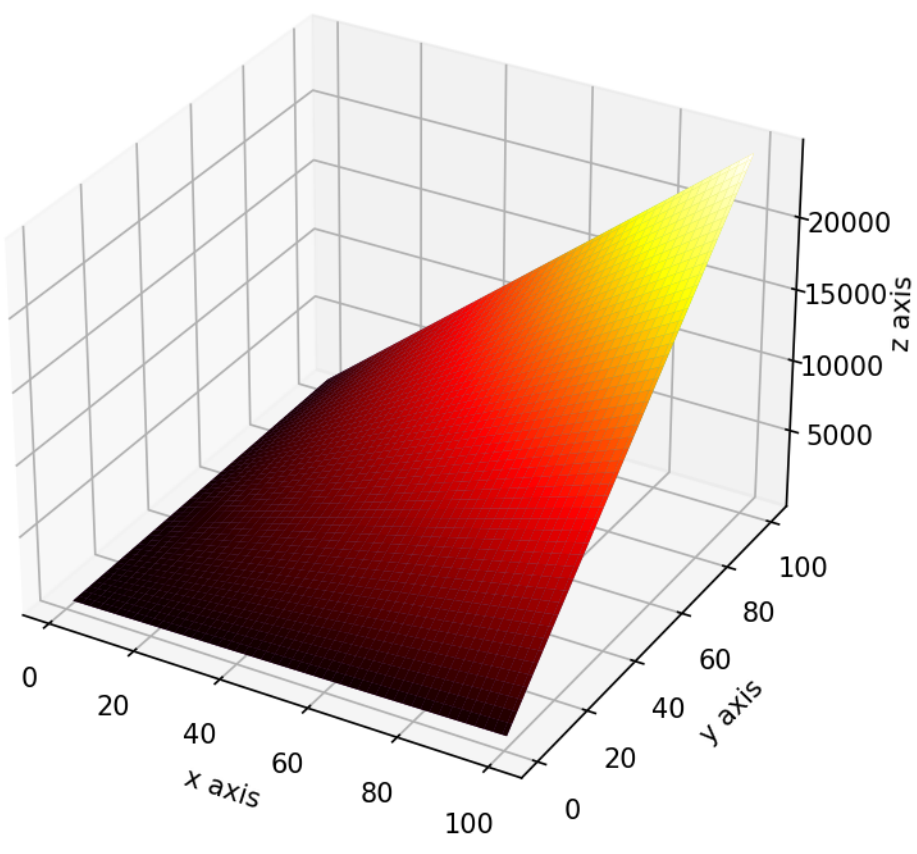
$$\begin{aligned} SCI &= \frac{6}{\sqrt{2+2}} + \frac{(8n-4)}{\sqrt{2+3}} + \frac{(2n-1)}{\sqrt{3+3}} \\ &= 3 + \frac{8n-4}{\sqrt{5}} + \frac{(2n-1)}{\sqrt{3}} \\ &= \frac{(8\sqrt{6}+2\sqrt{5})n-(4\sqrt{6}+\sqrt{5})}{\sqrt{30}}+3 \end{aligned}$$

When m > 1,

$$
\begin{aligned}
H &= \frac{(m+4)}{2} + \frac{2m+8n-4}{\sqrt{5}} + \frac{6mn-4n-m-1}{\sqrt{6}} \\
&= \frac{\sqrt{30}m + 4\sqrt{30} + 4\sqrt{6}m + 16\sqrt{6}n - 8\sqrt{6} + 12\sqrt{5}mn - 8\sqrt{5}n - 2\sqrt{5}m - 2\sqrt{5}}{2\sqrt{30}} \\
&= \frac{(\sqrt{30} + 4\sqrt{6} - 2\sqrt{5})m + (16\sqrt{6} - 8\sqrt{5})n + 12\sqrt{5}mn + (4\sqrt{30}\,8\sqrt{6} - 2\sqrt{5})}{2\sqrt{30}}
\end{aligned}
$$

□

fig 10 :Surface Plot of SCI



Result 8. The ABC Index of G is

$$
ABC(G) = \begin{cases} \dfrac{2+4\sqrt{2}}{3\sqrt{2}}n + (\sqrt{2}-2) & \text{if } m = 1, \\ \dfrac{(2\sqrt{2}-3)}{2}m + \dfrac{9-8\sqrt{2}}{\sqrt{2}}n - 4mn - \dfrac{2}{5} & \text{if } m > 1. \end{cases}
$$

Proof. ABC(G) = $\sum \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}$
When m = 1,

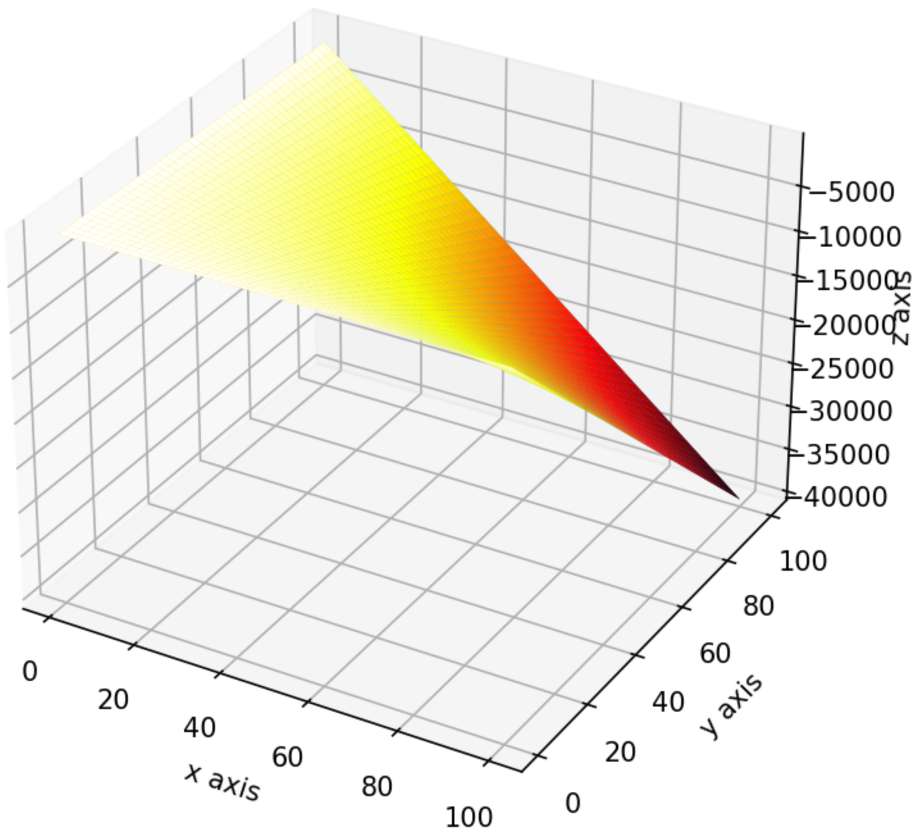
$$\begin{aligned}
ABC &= \frac{6}{\sqrt{2}} + \frac{(8n-4)}{\sqrt{2}} + \frac{2(2n-1)}{\sqrt{3}} \\
&= \frac{18 + 24n - 12 + 4\sqrt{2}n - 2\sqrt{2}}{3\sqrt{2}} \\
&= \frac{(2+4\sqrt{2})n + (6-2\sqrt{2})}{3\sqrt{2}} \\
&= \frac{2+4\sqrt{2}}{3\sqrt{2}}n + (\sqrt{2}-2)
\end{aligned}$$

When m $>$ 1,

$$\begin{aligned}
H &= \frac{(m+4)}{\sqrt{2}} + \frac{2m+8n-4}{\sqrt{2}} + \frac{2}{3}(6mn - 4n - m - 1) \\
&= \frac{3m + 12 + 6m + 24n - 12 + 12\sqrt{2}mn - 8\sqrt{2}n - 2\sqrt{2}m - 2\sqrt{2}}{3\sqrt{2}} \\
&= \frac{(6-2\sqrt{2})}{3\sqrt{2}}m + \frac{27-8\sqrt{2}}{3\sqrt{2}}n - \frac{12\sqrt{2}mn}{3\sqrt{2}} - \frac{2\sqrt{2}}{3\sqrt{2}} \\
&= \frac{(2\sqrt{2}-3)}{2}m + \frac{9-8\sqrt{2}}{\sqrt{2}}n - 4mn - \frac{2}{5}
\end{aligned}$$

□

fig 11 : Surface Plot of ABC



5 CONCLUSIONS

In this article, we have computed various degree based topological indices, like the Randic Index, the First and Second Zagreb Index, the Augmented Zagreb Index, the GA Index, the Harmonic Index, the Sum Connectivity Index and the Atom Connectivity Index of the graphene structure.

The Randic Index is correlated with physico chemical properties like boiling point, surface area, etc. where as ABC Index helps in the understanding of stability, strain energy, etc. GA Index has more predictive power than the Randic and ABC Indices. The First and Second Zagreb Indices occur in the computation of the total energy of molecules.

All the results in this paper are discussed graph theoretically, not experimentally. Computation of topological indices remain an open and challenging area for researchers. We hope that the results in this paper will provide a significant contribution to graph theory and correlate the chemical structure of graphene with a large amount of information about its physico chemical properties.

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