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

Research Article

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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-Polynomials

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 concept of 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 (12; 13; 21). They play an important role in the Quantitative Structure Activity Relationship (QSAR) and the Quantitative Structure Property Relationship (QSPR) (6; 12; 21). Many degree-based topological indices that correspond to chemical properties of the material under investigation are generated by M-polynomials.

A graph G (16) 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.

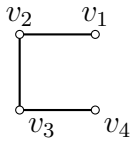


Fig. 1 An undirected graph G with four vertices and three edges

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 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) (16). In Fig. 1, v_1 and v_2 are adjacent while v_1 and v_3 are not.

Graphene is a two dimensional material derived from graphite, composed entirely of carbon atoms arranged in a hexagonal lattice. As a fundamental element in nature, carbon is ubiquitous in everyday materials, including the graphite found in pencil leads. Graphene is recognized as the world's thinnest, strongest, and most electrically and thermally conductive material. It is notable for its exceptional combination of toughness, flexibility, lightness, and high tensile strength. Studies estimate that graphene is approximately 200 times stronger than steel and five times lighter than aluminium. Because of these remarkable properties, it has a wide range of applications, including sensors, batteries, and carbon nanotubes. In addition, carbon-based materials such as carbon fibres play a critical role in the construction of modern aircrafts due to their strength-to-weight efficiency.

2 Literature Review and Motivation

Chemical graph theory has long been a powerful tool for modeling molecular structures using the principles of discrete mathematics. Among its most prominent tools are degree-based topological indices, which translate the connectivity of molecular graphs into numerical descriptors that correlate with physical and chemical properties (6).

In 2014, Gutman et al. (11) introduced the concept of the *M-polynomial* as a unifying method to compute a wide range of degree-based indices such as the Randić, Zagreb, GA, and ABC indices. This algebraic framework enables symbolic derivation of these indices once the edge distribution by vertex degrees is known. Since then several researchers have extended the M-polynomial method to model nanostructures. Murtaza et al. (19) applied it to graphene oxide, while Javaid et al. (17) analyzed graphene-like nanoribbons. Rafique et al. (20) demonstrated its applicability to silicate and hexagonal networks. These studies affirm the M-polynomial's flexibility and predictive power in capturing molecular behavior.

However, many of these works focus on specific classes of hydrocarbons, lattices, or chemically modified graphene derivatives. There remains a gap in the systematic application of M-polynomials to *pure finite graphene structures*, particularly with the aim of linking calculated indices to key molecular properties such as surface area, strain energy, and stability.

The exceptional electrical, thermal, and mechanical properties of Graphene are closely tied to its molecular structure. Topological descriptors offer a computationally inexpensive and structurally informative approach to approximating important physicochemical properties of molecular systems, making them valuable tools in theoretical chemistry and materials science. Motivated by this, the present work explores how the M-polynomials derived from degree-based indices can characterize finite graphene structures and correlate with their physicochemical behavior. By analyzing edge types and computing relevant indices, we hope that this study will contribute to the theoretical understanding of graphene and supports its application in materials science and nanotechnology.

3 Basic Definitions

In this section, we summarize several classical degree-based topological indices that are utilized in our analysis. These indices serve as mathematical descriptors of molecular structures and are extensively applied in chemical graph theory, particularly in the modeling of physicochemical properties through QSAR/QSPR studies.

1. **Randić Index:** Introduced by Milan Randić in 1975 (13), the Randić index of a graph G, denoted by $R(G)$, is defined as

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}},$$

where d_u and d_v denote the degrees of vertices u and v, respectively.

2. **Zagreb Indices:** Proposed by Trinajstić and Gutman in 1972 (12), the first and second Zagreb indices are given by:

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v), \quad M_2(G) = \sum_{uv \in E(G)} d_u \cdot d_v.$$

3. **Augmented Zagreb Index (AZI):** Defined by Furtula et al. in 2010 (9), the AZI index is expressed as:

$$AZI(G) = \sum_{uv \in E(G)} \left[\frac{d_u d_v}{d_u + d_v - 2} \right]^3.$$

4. **Geometric–Arithmetic Index (GA):** Introduced by Vukićević and Furtula in 2009 (22), the GA index is defined as:

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

5. **Harmonic Index (H):** Proposed by Zhong in 2012 (25), the harmonic index is defined as:

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}.$$

6. **Atom–Bond Connectivity Index (ABC):** Introduced by Estrada et al. in 1998 (7), the ABC index is defined as:

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u d_v}}.$$

Definition 3.1. M-polynomial of a graph G (5; 11)

Let $G = (V, E)$ be a graph. For $i, j \geq 1$, let $m_{i,j}$ denotes 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 is denoted by M(G; x, y) and 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.

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 (Fig. 2). This is taken as a single unit of graphene. Each vertex represents a carbon atom, and each edge a covalent bond. This structure is used as the building block in larger finite graphene graphs.

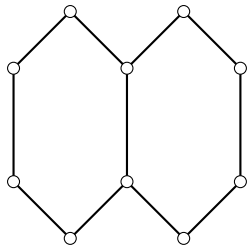


Fig.2 Basic unit of graphene represented as two fused hexagons sharing a common edge

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

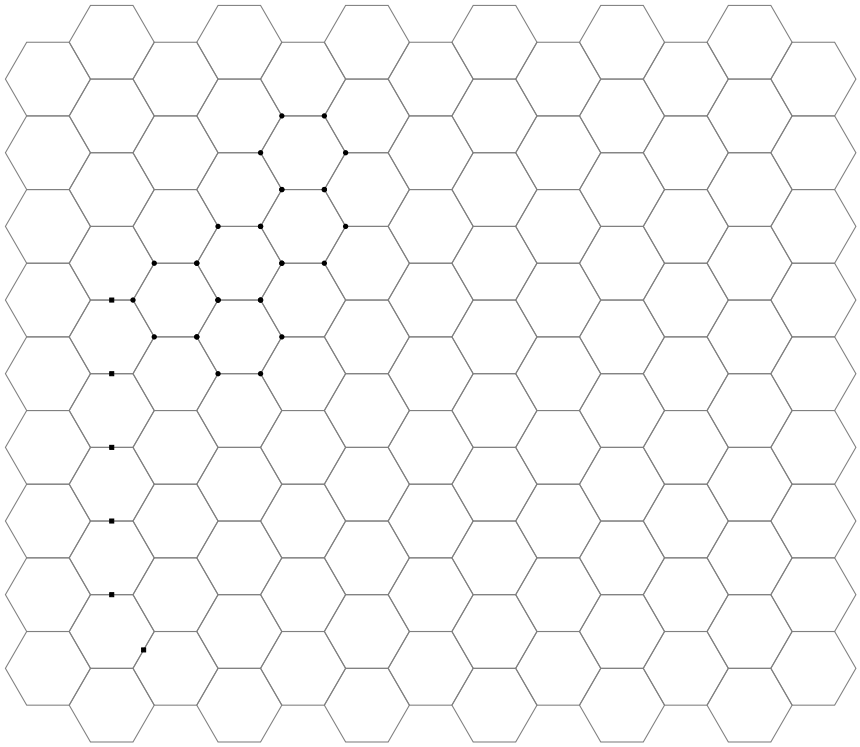


Fig. 3 A finite graphene nanostructure composed of $m \times n$ hexagonal units

3.1 Degree Distribution in Graphene

In an ideal infinite graphene sheet, every carbon atom is bonded to three others, forming a regular hexagonal tiling. Thus alll vertices have degree 3 and all edges connect two degree 3 vertices.

Therefore, the M-polynomial of an infinite sheet of graphene is

$$M(G; x, y) = m_{3,3} \cdot x^3 y^3$$

3.2 Edge Types in Graphene Structure

Table 1: Classification of Edge Types in Graphene Molecular Graphs

Edge Type	Description	Type of the graphene
$(3, 3)$	Internal edge between two degree-3 carbon atoms	Infinite and finite
$(2, 3)$	Edge between boundary vertex and interior vertex	Finite only
$(2, 2)$	Edge between two boundary (degree-2) vertices	Finite only (typically corners)

Thus the edges of a finite graphene are partitioned into (2, 2), (2,3) & (3,3) groups as follows.

Table 2: Edge partition in a finite (m,n) graphene

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 that G is a finite (m, n) chain of graphene. Using table 2, we define the M-polynomial of such a graphene as below.

Definition 3.2. M-polynomial of a finite (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. The M-polynomial corresponding to the Randic Index is given by

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

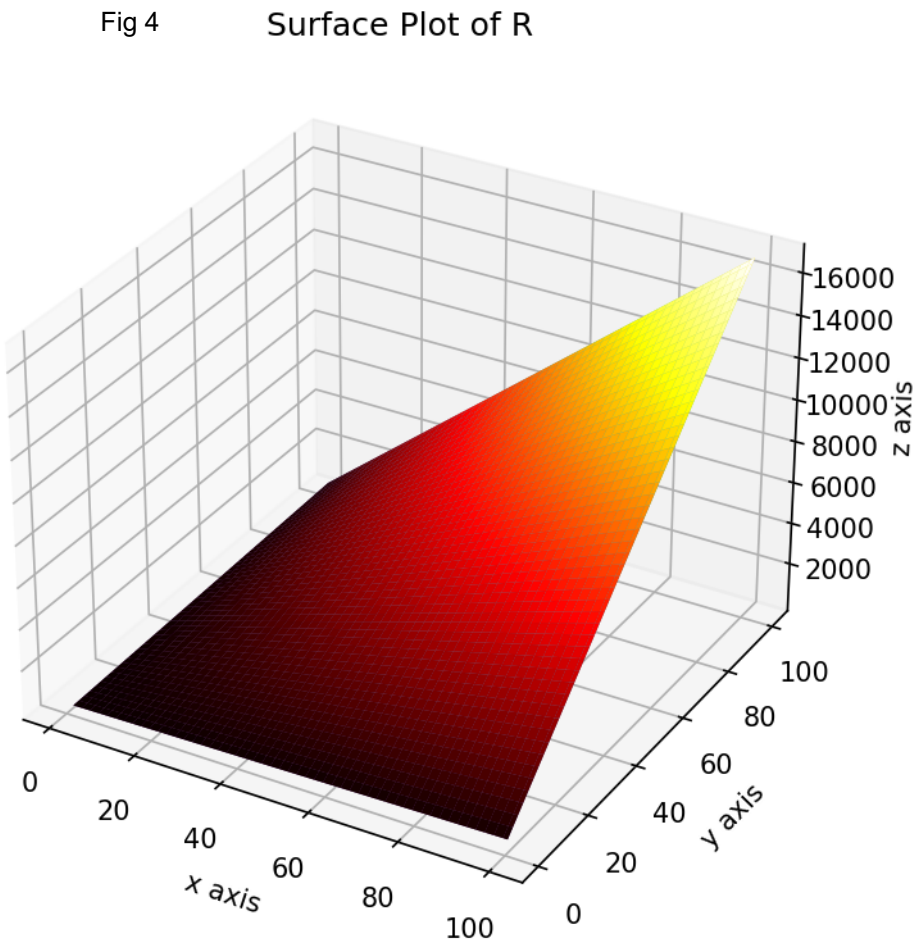
Proof. R(G) = $\sum_{uv \in E} \dfrac{1}{\sqrt{d_u d_v}}$
When m = 1

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

When m $>$ 1

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

Fig 4



□

Result 2. The M-polynomial corresponding to the first Zagreb Index of G,

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

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

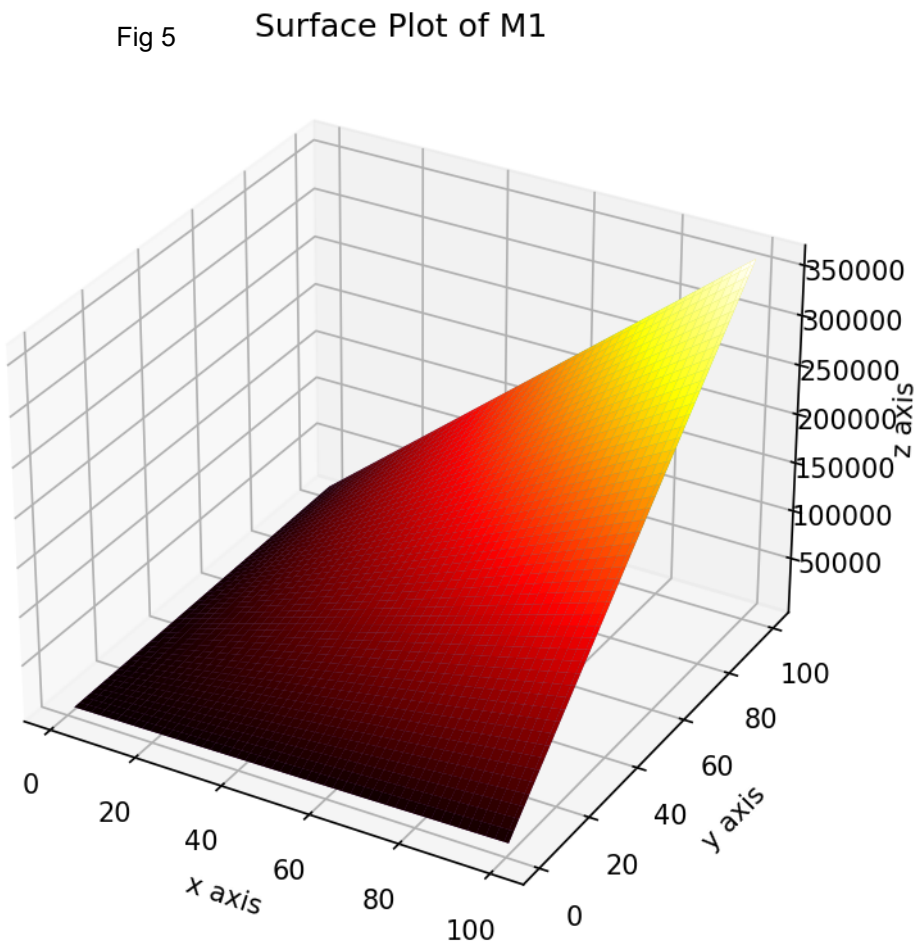
$$\begin{aligned} M_1(G) &= 6(2+2) + (8n-4)(2+3) + (2n-1)(3+3) \\ &= 24 + 40m - 20 + 12n - 6 \\ &= 52n - 26 \\ &= 26(2n-1) \end{aligned}$$

When m $>$ 1

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

□

Fig 5



Result 3. The M-polynomial corresponding to the second Zagreb Index of G,

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

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

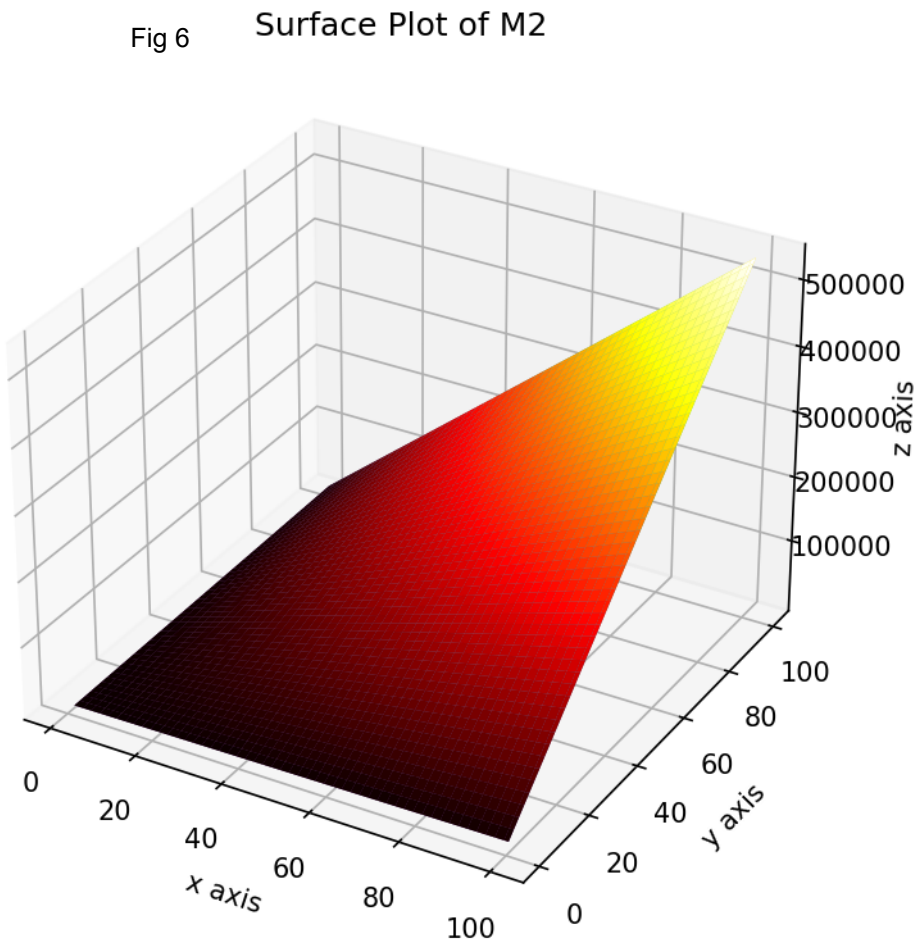
$$\begin{aligned} M_2(G) &= 6(2.2) + (8n-4)(2.3) + (2n-1)(3.3) \\ &= 24 + 48n - 24 + 18n - 9 \\ &= 66n - 9 \end{aligned}$$

When m $>$ 1

$$\begin{aligned} M_2(G) &= (m+4)(2.2) + (2m+8n-4)(2.3) + (6mn-4n-m-1)(3.3) \\ &= 4m + 16 + 12m + 48n - 24 + 50mn - 36n - 9m - 9 \\ &= 7m + 12n + 54mn - 17 \end{aligned}$$

□

Fig 6



Result 4. The M-polynomial corresponding to the Augmented Zagreb Index of G is

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

Proof. AZI(G) = $\sum \left[\dfrac{d_u d_v}{d_u + d_v - 2}\right]^3$

When m = 1,

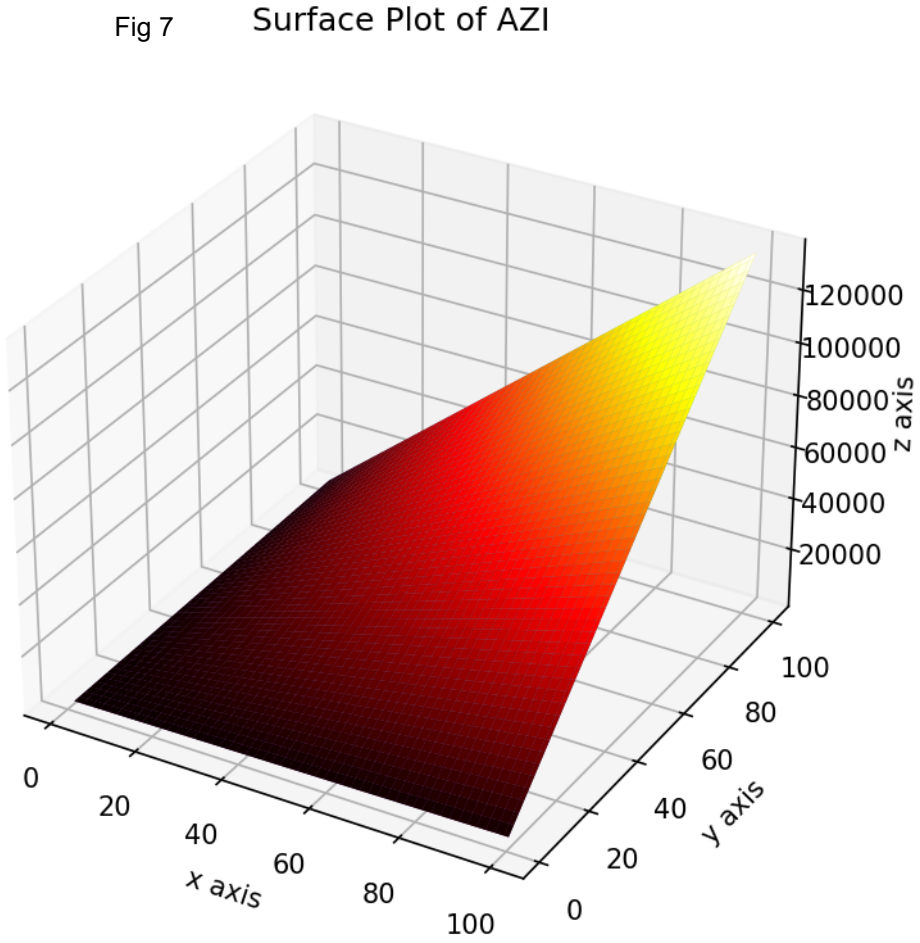
$$\begin{aligned} AZI(G) &= 6\left[\frac{2.2}{2+2-2}\right]^3 + (8n-4)\left[\frac{2.3}{2+3-2}\right]^3 + (2n-1)\left[\frac{3.3}{3+3-2}\right]^3 \\ &= \frac{82n+7}{4} \end{aligned}$$

When m $>$ 1,

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

□

Fig 7



Result 5. The M-polynomial corresponding to 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,

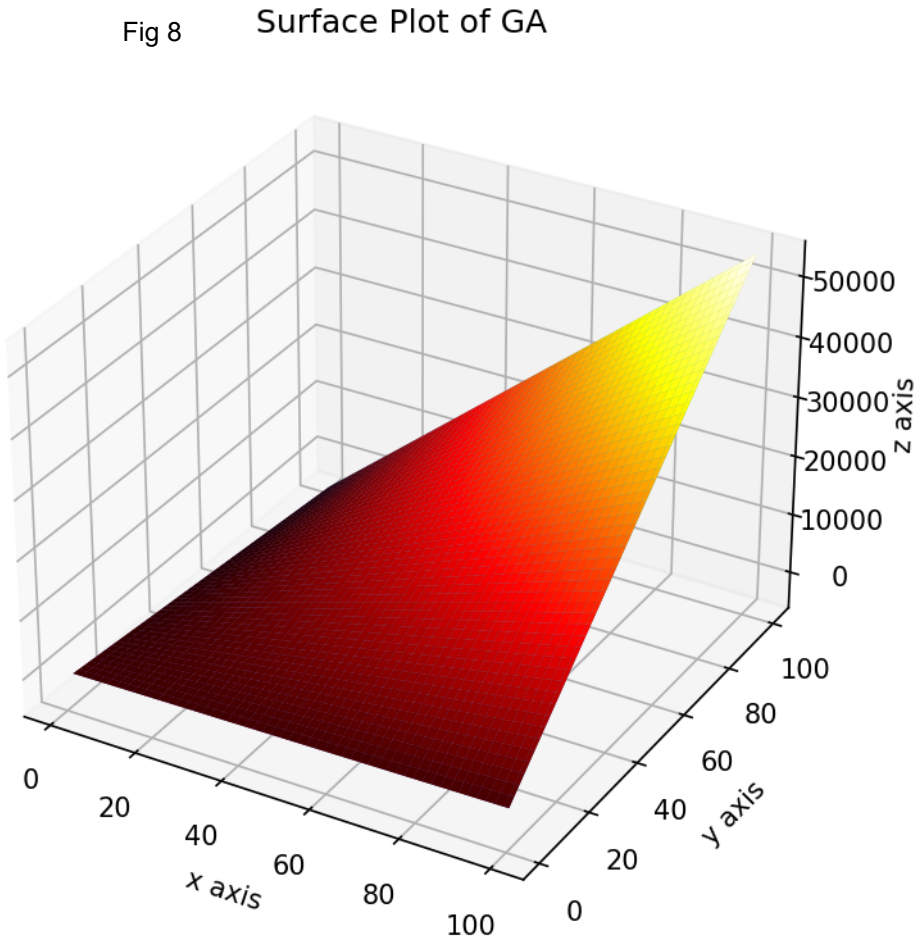
$$\begin{aligned} GA(G) &= 6\frac{2\sqrt{4}}{4} + (8n-4)\frac{2\sqrt{6}}{5} + (2n-1)\frac{2\sqrt{9}}{6} \\ &= 6 + \frac{2\sqrt{6}}{5}8n - 4\frac{2\sqrt{6}}{5} + (2n-1) \\ &= \frac{1}{5}\left[(16\sqrt{6}+10)n + (25-8\sqrt{6})\right] \end{aligned}$$

When m $>$ 1,

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

□

Fig 8



Result 6. The M-polynomial corresponding to the Harmonic Index of G is

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

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

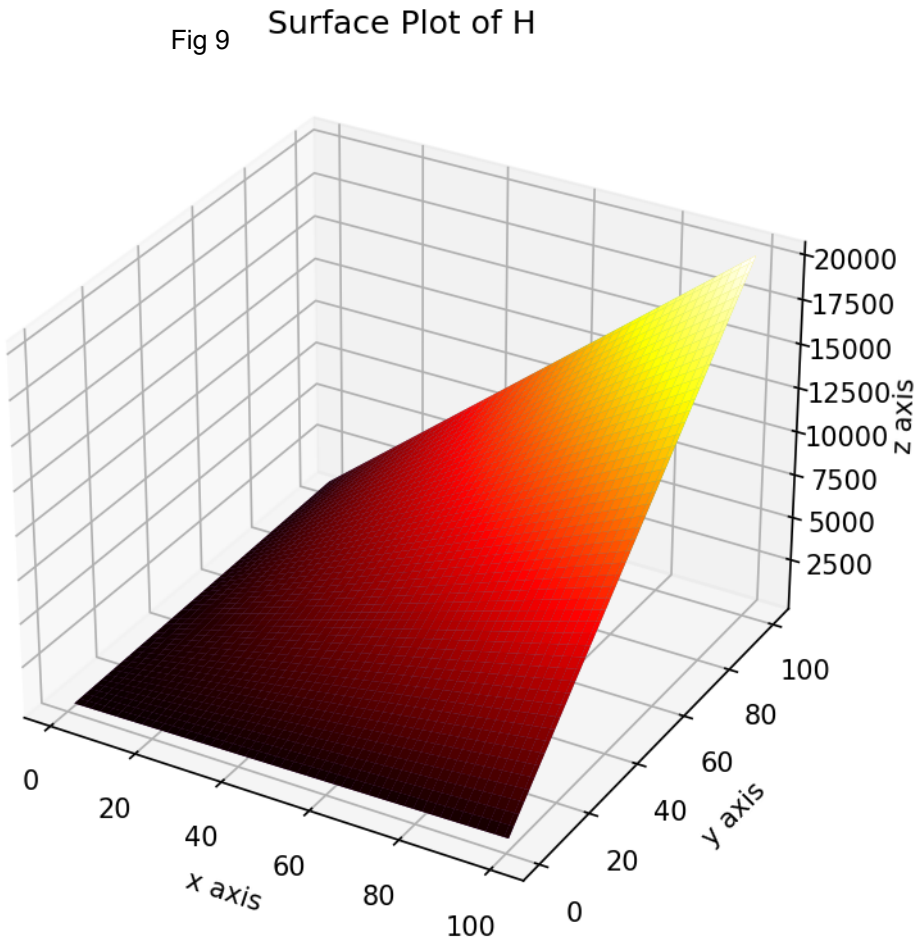
$$\begin{aligned} H(G) &= 6\frac{2}{2+2} + (8n-4)\frac{2}{2+3} + (2n-1)\frac{2}{3+3} \\ &= \frac{6}{2} + \frac{16n-8}{5} + \frac{(2n-1)}{3} \\ &= \frac{90+96n-48+20n-10}{30} \\ &= \frac{116n+32}{30} \\ &= \frac{58n+16}{15} \end{aligned}$$

When m $>$ 1,

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

□

Fig 9



Result 7. The M-polynomial corresponding to 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) = $\sum \frac{1}{\sqrt{d_u+d_v}}$

When m = 1,

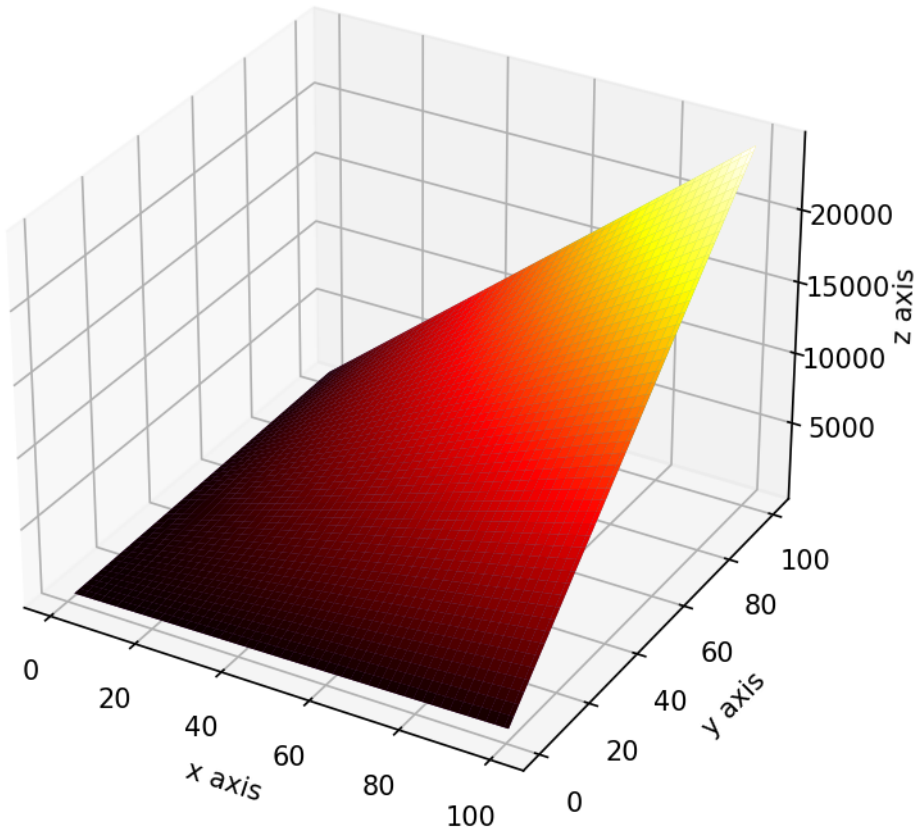
$$\begin{aligned} SCI(G) &= \frac{6}{\sqrt{2+2}}+\frac{(8n-4)}{\sqrt{2+3}}+\frac{(2n-1)}{\sqrt{3+3}} \\ &= 3+\frac{8n-4}{\sqrt{5}}+\frac{(2n-1)}{\sqrt{3}} \\ &= \frac{(8\sqrt{6}+2\sqrt{5})n-(4\sqrt{6}+\sqrt{5})}{\sqrt{30}}+3 \end{aligned}$$

When m $>$ 1,

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

□

Fig 10 Surface Plot of SCI



Result 8. The M-polynomial corresponding to the ABC Index of G is

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

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

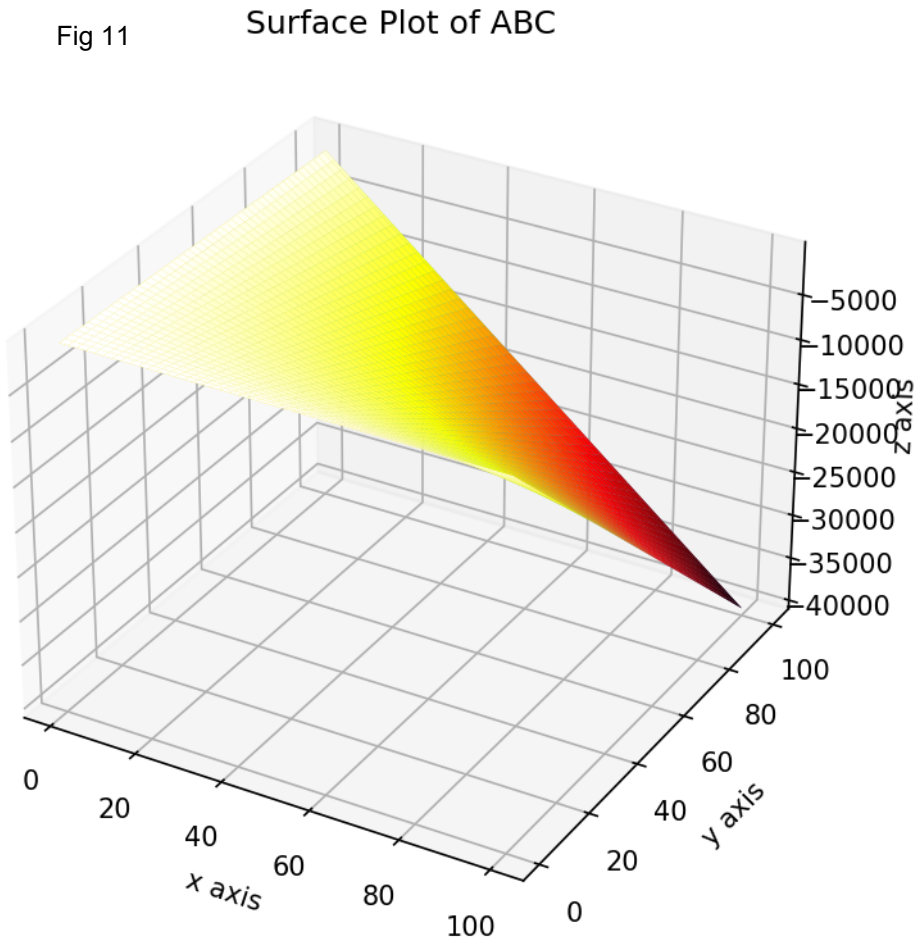
$$\begin{aligned} ABC(G) &= \frac{6}{\sqrt{2}} + \frac{(8n-4)}{\sqrt{2}} + \frac{2(2n-1)}{\sqrt{3}} \\ &= \frac{18 + 24n - 12 + 4\sqrt{2}n - 2\sqrt{2}}{3\sqrt{2}} \\ &= \frac{(2+4\sqrt{2})n + (6-2\sqrt{2})}{3\sqrt{2}} \\ &= \frac{2+4\sqrt{2}}{3\sqrt{2}}n + (\sqrt{2}-2) \end{aligned}$$

When m $>$ 1,

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

□

Fig 11



6. Comparative Analysis with Physicochemical Properties of Graphene

In this section, we compare the calculated indices for small graphene-like structures (with increasing number of hexagonal units) with representative molecular descriptors such as estimated surface area and strain energy. While precise experimental data for graphene flakes varies, approximate trends provide insight into the predictive utility of the topological indices.

The calculated degree-based topological indices offer useful predictors for several key physicochemical properties of graphene. The Randić index, which decreases with increasing branching, is known to correlate inversely with molecular surface area. The ABC index, which quantifies atomic bond connectivity, has shown strong correlation with molecular strain and thermodynamic stability. The GA index, combining geometric and arithmetic means of vertex degrees, has demonstrated greater predictive power in QSPR studies. The First and Second Zagreb Indices appear in energy calculations, particularly in the estimation of total π-electron energy for conjugated systems such as graphene. They scale quadratically with structure size, reflecting total degree-weighted connectivity and energy

Table 3: Comparison of Degree-Based Topological Indices with Molecular Descriptors of Finite Graphene Nanostructures

Size $(m \times n)$	**R**	**GA**	**ABC**	$\mathbf{M}_1$	$\mathbf{M}_2$	**AZI**	**H**	**SCI**	**Area (nm^2)**	**Strain (kJ/mol)**
1×1	5.62	7.91	6.44	26	57	22.5	4.32	4.84	0.52	60.2
2×2	13.41	18.72	15.26	102	223	70.6	10.27	11.34	1.04	55.7
3×3	25.23	34.59	29.78	234	515	157.8	18.65	20.81	1.57	52.4
4×4	40.10	56.82	48.21	410	903	284.2	29.42	32.34	2.09	50.1

contributions. The Harmonic Index captures bond equilibrium and is useful in estimating molecular symmetry. The Sum Connectivity Index helps assess local structural compactness and correlates with melting and boiling points.

As shown in Table 3, each index exhibits a monotonic growth trend with increasing molecular size. These comparisons validate the chemical relevance of the computed topological descriptors and their potential utility in the predictive modeling of graphene-based materials.

5 CONCLUSIONS

In this article, we investigated the structural and chemical characteristics of graphene through the lens of topological graph theory. Applying the M-polynomial framework, we computed several key degree-based topological indices, namely the Randić index, the ABC index, the GA index and the first and second Zagreb indices, for finite fragments of graphene modeled as an (m, n) chain.

Our analysis revealed significant correlations between these topological descriptors and important physicochemical properties of graphene, including surface area and strain energy. The M-polynomial method provided a unified and efficient approach to derive these indices from the graph's edge degree distribution. We also demonstrated how these indices scale with increasing graphene size and reflect predictable trends in molecular behavior.

Furthermore, a comparative evaluation with known molecular descriptors confirmed the relevance of the selected indices in the context of Quantitative Structure–Property Relationships (QSPR). This reinforces the applicability of M-polynomial based descriptors in theoretical chemistry and materials science.

All the results in this paper are discussed graph theoretically, not experimentally. The computation of topological indices remains an open and challenging area for researchers. We hope that the results in this paper will provide a significant contribution to graph theory and will correlate the chemical structure of graphene with a large amount of information about its physicochemical properties. Future work may explore the extension of this approach to graphene derivatives, nanoribbons, and periodic structures using weighted or edge-decorated graphs. Integration with machine learning models may further enhance the predictive power of these indices for material designs and property forecasting.

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