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COUNTING POLYNOMIALS AND ASSOCIATED TOPOLOGICAL INDICES OF NANOGRAPHENE AND TRIANGULAR NANOGRAPHENE WITH PENDANT EDGES: A PYTHON-BASED COMPUTATIONAL FRAMEWORK

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Abstract: *In this paper, Nanographene with pendant edges and Triangular nanographene with pendant edges are investigated for general dimension γ using graph-theoretical methods. Edge distances are calculated by applying acute cuts, middle cuts, and pendant edge cuts. Based on these distances, derived four specific counting polynomials namely, the Omega(Ω), Theta(θ), Pi(π), and Sadhana(Sd) polynomials , and the subsequent indices are obtained for both classes of structures. These polynomials are examined in relation to their underlying physical structure, giving information on topological variation, electronic movement, and possible chemical uses. The theoretical knowledge of chemically significant nanostructures is improved by this work, which also creates opportunities for modeling their behavior using polynomial invariants. In addition, Python-based algorithms are proposed to generate the both structures for any dimension and to compute the associated polynomials and indices efficiently. The computational results are consistent with the theoretical findings, confirming the correctness of the approach. The proposed methodology enables rapid computation, producing results within a very short time, and gives an effective framework for analyzing nanographene structures with pendant edges.*

Keywords: *Nanographene, Triangular nanographene, Pendant edges, Graph polynomials, Omega (Ω) polynomial, Theta (θ) polynomial, Pi (π) polynomial and Sadhana (Sd) polynomial, indices.*

1 Introduction

Graphene and its derivatives, such as nanographene systems, have attracted a lot of attention because of its symmetrical structure and electrical adaptivity. Significant spectral and topological changes are observed in these type of systems when pentagonal edge distortions, which is called as pendant edges are introduced into the new standard hexagonal frames. Graph-theoretical methods provide an effective framework for modeling such structures, where molecular systems are represented as graphs and analyzed using suitable mathematical descriptors [26, 32].

The four Counting polynomials, such as Omega(Ω), Theta(θ), Pi(π), and Sadhana(Sd) polynomials play an important role in characterizing structural properties related to edge distances and connectivity patterns. These polynomials further lead to the computation of subsequent indices, which are useful in understanding molecular stability and predicting physicochemical properties [8, 24]. Although these concepts have been studied for various molecular structures, systematic investigations for nanographene and triangular nanographene with pendant edges remain largely unexplored.

In this study, we focus on Nanographene and Triangular nanographene structures with pendant edges of arbitrary dimension γ. By applying different edge-cut techniques, namely acute cuts, middle cuts, and pendant edge cuts, edge distances are calculated and subsequently used to derive the four Counting polynomials, such as Omega(Ω), Theta(θ), Pi(π), and Sadhana(Sd) polynomials and the subsequent indices. Furthermore, Python-based algorithms[1] are developed

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to generate these structures for any dimension and to findout the polynomials and indices within a very short computational time (typically less than 10 seconds). This efficient approach enables rapid analysis and supports further studies of Nanographene and Triangular nanographene systems with pendant edges.

Novelty of the Work

This study deals with the construction of nanographene and triangular nanographene structures with pendant edges and the analysis of their associated counting polynomials. Earlier studies have investigated counting polynomials for graphene-based systems, including supercoronenes and triangular discotic graphene [27], as well as the structural characteristics and properties of nanographene materials [32]. However, these works are mainly limited to standard structures and do not take into account the effect of pendant edge modifications. In the present work, new nanographene models with pendant edges are introduced, and explicit expressions for Omega, Theta, Pi, and Sadhana polynomials, along with their corresponding topological indices, are obtained. Further, a Python-based computational framework is developed to generate these structures for any dimension n and to compute the corresponding polynomials and their derivatives efficiently. Thus, the proposed approach not only extends existing theoretical results but also offers a practical and scalable method for studying complex nanographene systems.

2 Preliminaries and Structural Description

Graph theory is practised to examine the hard molecules like graphene, taking atoms as points (vertices) and the bonds that connects atoms as connections (edges). By using this way, we can able to formulate the mathematical expressions using edge partitions known as counting polynomials that gives the information about the relationships between edges, particularly with respect to their distances and connectivity patterns [26].

Carbon atoms are systematic arrangement in a two-dimensional honeycomb pattern to form the graphene and its derivatives of the graphene [26]. These are the exciting elements, due to their structural, chemical, and electrical characteristics. In particular Nanographenes are very interesting concepts because of their characteristics can vary significantly based on their size , structure or modification of their edges [25].

A finite piece of graphene is shown in the Figure 1 as a two dimensional honeycomb lattice of sp^2 carbon atoms with dimension $\gamma = 4$ [6, 32]. It shows nanographene, where outer atoms are fixed through termination, as a cuts from the infinite graphene sheet. A number of outer sites extend as pendant edges, which may signal structural flaws or acts as locations for chemical functionalization[22]. These edge changes are essential for adjusting the nanographene's electrical, magnetic, and reactive characteristics. Therefore, the schematic serves as a link between the topological descriptors used in the prediction of chemical properties and the molecular structure[29].

The nanographene fragment of the symmetric polycyclic aromatic hydrocarbon circumcoronene $C_{96}H_{12}$ shown in Figure 1 [29]. A hexagonal honeycomb lattice of carbon atoms makes up its structure, with hydrogen atoms capping each carbon edge to remove dangling

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connections and stabilize the molecule, the general form of the Nanographene with pendant edges is denoted as $C_{6n^2}H_{6n}$. Because it is made up of fused benzene rings and maintains as extended delocalized Π-electron system, circumcoronene is a great chemical counterpart of bulk graphene [23].

In computational chemistry, circumcoronene is frequently employed as a tractable graphene model to investigate noncovalent interactions such as molecule adsorption and $\Pi - \Pi$ stacking. Because of its size, the core region can simulate the electrical environment of infinite graphene while yet being computationally reasonable such that benzene adsorption on nanographene results in binding energies of about $-41\text{kJ} \cdot \text{mol}^{-1}$ [23].

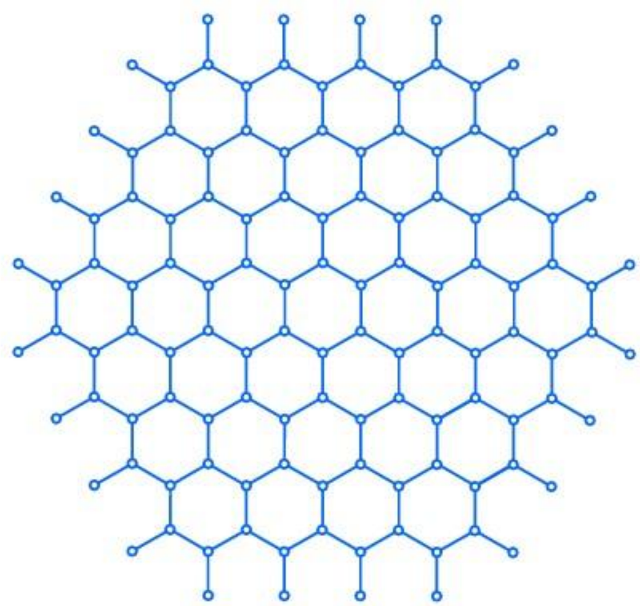

Figure 1: Nanographene with Pendant Edges of Dimension $\gamma = 4$

A triangular nanographene lattice made from graphene is shown in the Figure 2 , highlighted the geometric variety of edge patterns. To extent outword from the vertices and sides which are called as the pendant edges, which could be the locations for molecular attachment or chemical alteration. In contrast to the typical hexagonal graphene pieces, this triangular geometry introduces unique edge states an quantum confinement effects, the pendent edges and triangle shape work together to improve the tunability of chemical, optical, magnetic, and electrical characteristics[29]. Topological descriptors, which connect shape to function, are crucial for designing materials and nanoscale electronics.

The finite triangular graphene nanoflake (GNF) with zigzag edges shown in Figure 2 is commonly referred to as a triangulene or, more broadly, an γ-triangulene in the literature. Hydrogen atoms terminate the edge carbons, which are seen as tiny peripheral groups, and the carbon atoms in this configuration create a triangular array of fused benzene rings. The flake in the illustration has the formula $C_{33}H_{15}$, which is equivalent to a 5-triangulene (five hexagons per edge).In general of the γ triangulate is denoted as $C_{n^2+4n+1}H_{3n+3}$. This polycyclic aromatic

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hydrocarbon's (PAH) distinct molecular geometry is emphasized by its triangular symmetry and regular edge termination [7].

Though their zigzag edges localize unpaired electrons, triangular nanographenes chemically maintain a fully delocalized Π-electron cloud. An γ-triangulene ground state has a substantial open-shell feature due to its roughly $(\gamma - 1)$ unpaired electron count. Because of the concentration of these unpaired spins at the edges, strongly correlated electronic states, magnetic ordering, and radical characteristics are produced. Reduced HOMO-LUMO gaps and improved quantum confinement result from the polyradical nature growing as the size parameter γ increases[7].

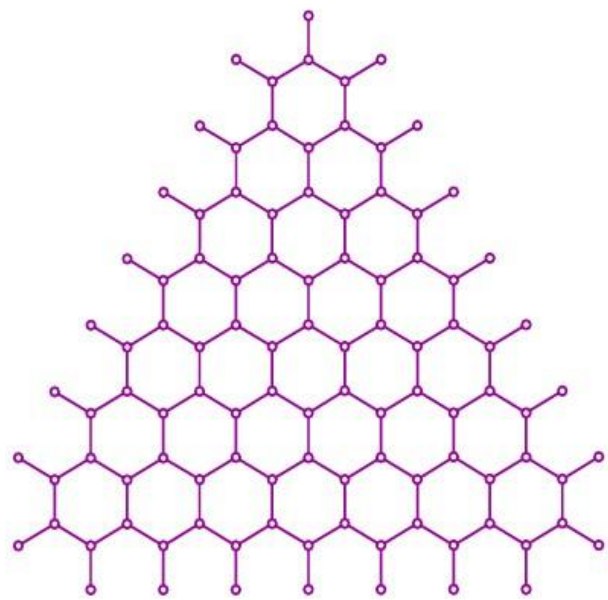

Figure 2: Triangular Nanographene with Pendant Edges of Dimension $\gamma = 7$

In this paper, we focus on Nanographene and Triangular nanographene structures with extra miniature connections, known as pendant edges, which are efficiently extra edges connected to specific molecules. These pendent edges have a major impact on the structure and, consequently, the behavior of the material.

3 Methodology

The proposed methodology follows a systematic framework for analyzing Nanographene and Triangular nanographene structures with pendant edges for a given dimension γ. Initially, the base structures are constructed, starting from a fixed dimension and then generalized to arbitrary γ.

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Afterthat, the edge sets of the constructed graphs are classified using three types of edge-cut techniques, namely acute cuts, middle cuts, and pendant edge cuts. These edge cut technique is enable to understanding of the graph and facilitate the identification of edge-distance. Based on this classification, the ranges of edge distances are analyzed, and the corresponding number of edges in each category is determined. Based on these distances, derived four specific polynomials namely, the Omega(Ω), Theta(θ), Pi(π), and Sadhana(Sd) polynomials. From these polynomials, the corresponding topological indices are then derived using their standard definitions. To support the theoretical results, Python code [31] is developed to generate the corresponding graph structures for different dimensions. In addition, based on the derived polynomial expressions, the code is designed to efficiently compute the associated counting polynomials and topological indices for any given dimension n. The computational outputs are then compared with the theoretical results to verify their correctness and consistency. A clear overview of the methodology followed in this study is presented through the flowchart shown in Figure 3.

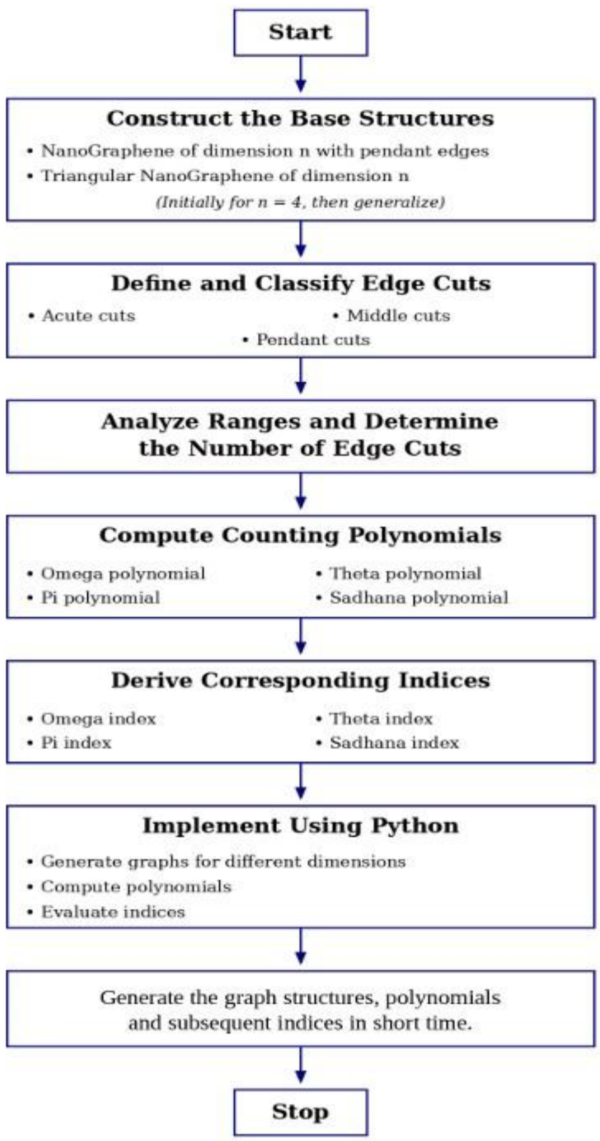

Figure 3: A flow chart

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. .

4 Counting Polynomials and Topological Indices

Let $G(V,E)$ be a connected molecular graph, with the edges $e_1 = u_1v_1$ and $e_2 = u_2v_2$ in the edge set $E(G)$ are called codistant (e_1coe_2) if $d(v_1,u_2) = d(v_1,v_2) + 1 = d(u_1,u_2) + 1 = d(u_1,v_2)$. Where $d(v_1,u_2)$ represents the distance between the edges v_1 and u_2. If the edges $e_1 = u_1v_1$ and $e_2 = u_2v_2$ satisfies the following relations reflexive, symmetric and transitive under codistant then its called an equivalence relation. [2, 20]

1. Reflexive $e_1 \ co \ e_1$
2. Symmetric $e_1 \ co \ e_2 \Leftrightarrow e_2 \ co \ e_1$
3. Transitive $e_1 \ co \ e_2 \ \& \ e_2 \ co \ e_3 \Rightarrow e_1 \ co \ e_3$

Though the third relation Transitive is not always valid [8].

If the set $C_i(e_1) = e_2, i = 1,2,\dots,\gamma$ should be the edge set in G, is orthogonal cut of the graph G then the relation codistant is transitive. If the graph G is called cograph then the edge set $E(G)$ is the union of disjoint orthogonal cuts and vice versa. That is, $E(G)$= $C_1 \cup C_2 \cup \dots \cup C_{k-1} \cup C_k$ such that $C_i \cap C_j = \varnothing \quad$ for all$i \neq j, \quad i,j \in \{1,2,\dots,k\}$.[21]

If the two successive edges of an edge which cuts the edges satisfying the reflexive and symmetric conditions then its called the quasi-orthogonal cut qoc. Using these qoc, in the year 2006 M.V Diudea [8] introduced the Omega polynomial which as

$$\Omega(G,x) = \sum_c m \cdot x^c$$

Let $m(G,c) = m$ be the number of qoc strips of length c and summation goes up the maximum length of qoc strips in G[10][9]. using the qoc, in the year 2008 Ashrafi at al. [5] proposed the Theta polynomial which as

$$\Theta(G,x) = \sum_c m \cdot c \cdot x^c$$

Omega and Theta polynomials counting the equidistant edges in G, Using the qoc, in the year 2008 Ashrafi at al. and Diudea [5] joined together to introduce the PI Polynomial which

$$\Pi(G,x) = \sum_c m \cdot c \cdot x^{e-c}$$

Where e represents the total number of edges of the graph G. PI polynomial counting the non equidistant edges in G.Also using the qoc, in the year 2008 Ashrafi at al. [3, 11, 19] proposed the Sadhana polynomial which as

$$Sd(G,x) = \sum_c m \cdot \ x^{e-c}$$

.

These counting polynomials are more helpful to the topological description of Graphene and Nanographene with pendant edges. The condition means both endpoints of one edge are at exactly the same distance from both endpoints of another edge. $d(u_1,x_1) = d(u_1,y_1) = d(v_1,x_1) = d(v_1,y_1)$. In the above counting polynomials,the first order derivative at $x = 1$, gives

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the indices of these polynomials. Which are called by Omega index, Theta index, Pi index [24] and Sadhana index and denoted symbolically [4]

$$\text{Omega index } \Omega(G) = (\Omega'(G,x))_{x=1} = (\sum_c m \cdot c x^{c-1})_{x=1} = |E(G)|$$

$$\text{Theta index } \theta(G) = (\Theta'(G,x))_{x=1} = (\sum_c m \cdot c \cdot c x^{c-1})_{x=1}$$

$$\text{Pi index } PI(G) = (\Pi'(G,x))_{x=1} = (\sum_c m \cdot c \cdot (e-c) x^{(e-c)-1})_{x=1}$$

$$\text{Sadhana index } Sd(G) = (Sd'(G,x))_{x=1} = (\sum_c m \cdot (e-c) x^{(e-c)-1})_{x=1}$$

From the Omega and Theta polynomials P.V. Khadikar to find the Pi index.

$PI(G) = e^2 - \sum m \cdot c^2 = [\Omega'(G,x)]^2 - \Theta'(G,x)_{x=1}$ [8] [20]

The Cluj-Ilmenau index [11], denoted by $CI(G)$, and is defined from the Omega polynomial [8] as:

(i) $CI(G) = [\Omega'(G,x)]^2 - [\Omega'(G,x) + \Omega''(G,x)]_{|x=1}$.
(ii) In planer bipartite graphs $CI(G) = PI(G)$[16] .
(iii) Pi index is calculated from the Omega and Theta polynomials[24].

$$\Pi'(G,1) = \Omega'(G,1) - \Theta'(G,1)$$

(iv) Sadhana index is also calculated from Omega polynomial[5]

$$Sd'(G,1) = [\Omega'(G,1)][\Omega(G,1) - 1]$$

5 Computational Results and Python Implementation

. In this section, we determine derived four specific polynomials namely, the Omega(Ω), Theta(θ), Pi(π), and Sadhana(Sd) polynomials , and the subsequent indices for Nanographene and Triangular Nanographene with pendant edges of dimension γ. The results are obtained using the edge classifications derived through acute cuts, middle cuts, and pendant edge cuts.

Theorem 1

Let G_1 Nanographene with pendant edges of dimension γ for $\gamma \geq 1$, Then,

1. $\Omega(G_1,x) = 6\left(\frac{x^{2\gamma} - x^{\gamma+1}}{x-1}\right) + 3x^{2\gamma} + 6\gamma x$

2. $\Theta(G_1,x) = 6\left(\frac{\gamma x^{\gamma+1}(x^{\gamma-1}-1)}{x-1} + \frac{x^{\gamma+1}(1-\gamma x^{\gamma-1}+(\gamma-1)x^{\gamma})}{(x-1)^2}\right) + 6\gamma x^{2\gamma} + 6\gamma x$

3. $\Pi(G_1,x) = 6\,x^{9\gamma^2+2\gamma}\left(\frac{\gamma(1-x^{-(\gamma-1)})(x-1)+x(1-\gamma x^{-(\gamma-1)}+(\gamma-1)x^{-\gamma})}{(x-1)^2}\right) + 6\gamma\,x^{9\gamma^2+\gamma} + 6\gamma\,x^{9\gamma^2+3\gamma-1}$

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4. $Sd(G_1,x) = 6\left(\frac{x^{9\gamma^2+2\gamma} - x^{9\gamma^2+\gamma+1}}{x-1}\right) + 3x^{9\gamma^2+\gamma} + 6\gamma x^{9\gamma^2+3\gamma-1}$.

Proof. The acute edges (A-type) of Nanographene with pendant edges ($\gamma = 4$) is divided into three groups in Figure 4. The three groups are acute edges (A-type)[15] have symmetry about the middle edges (M-type). We therefore count six times in order to determine the counting polynomials in A-type classes. And the middle cuts count 3 times. Then take the pendant edge, each counts as one and the number of times as 6γ. As a result, we can find the counting polynomial equations from the graph theoritical parameters shown in Table 1. The graph Graphene and Nano graphene system with pendant edges of dimension γ, total number of edges is $9\gamma^2 + 3\gamma$ [14, 33].

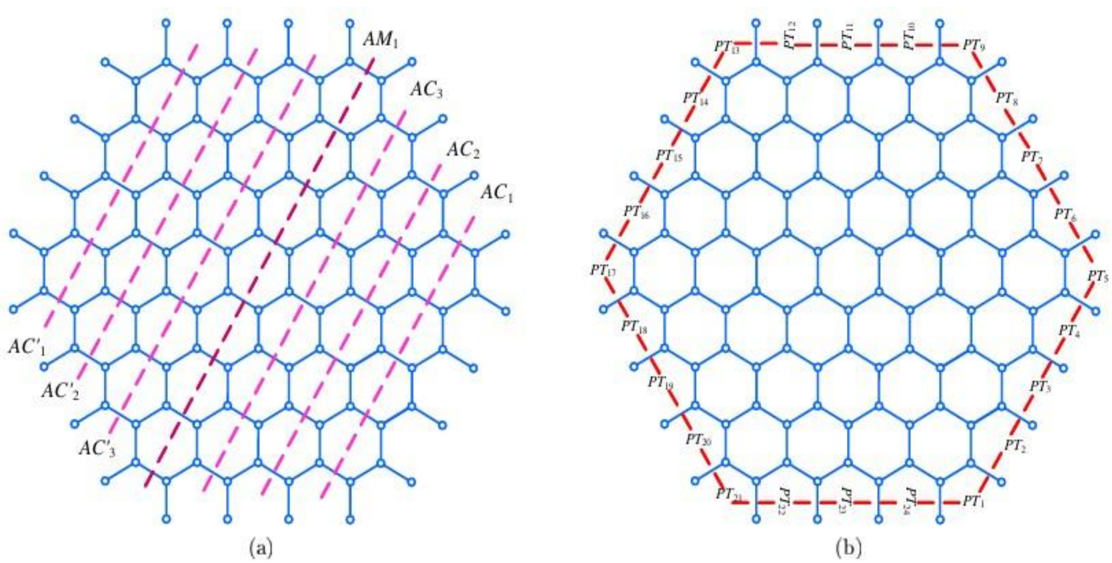

Figure 4: G_1 Nanographene with pendant edges of dimension 4 (a) G_1 acute cuts AC_i, and Middle cut AM_i (b) G_1 pendant edge cuts PT_i

From the structure shown in Figure 4, the edge partitions and their corresponding frequencies are listed in Table 1.

Type of Cuts	Ranges	Number of edges	Cut ordinality
$G_1/_{AC_i}$	$1 \le i \le (\gamma - 1)$	$\gamma + i$	6
$G_1/_{AM}$	1	2γ	3
$G_1/_{PT}$	1	1	6γ

Table 1: Edge partitions of Nanographene system with pendant edges of dimension γ.

Using the values given in Table 1 and applying the definition of Omega(Ω), Theta(θ), Pi(π), and Sadhana(Sd) polynomials, the required expression is obtained as follows.

$$\Omega(G_1,x) = \sum_c m \cdot x^c$$
$$= 6\sum_{k=1}^{\gamma} x^{\gamma+k} + 3x^{2\gamma} + 6\gamma x$$

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$$= 6\left(\frac{x^{2\gamma}-x^{\gamma+1}}{x-1}\right) + 3x^{2\gamma} + 6\gamma x$$

$$\Theta(G_1,x) = \sum_c m\cdot c\cdot x^c$$

$$= 6\sum_{k=1}^{\gamma-1} (\gamma+k)x^{\gamma+k} + 6\gamma x^{2\gamma} + 6\gamma x$$

$$= 6\left(\frac{\gamma x^{\gamma+1}(1-x^{\gamma-1})}{1-x} + \frac{x^{\gamma+1}(1-\gamma x^{\gamma-1}+(\gamma-1)x^{\gamma})}{(1-x)^2}\right) + 6\gamma x^{2\gamma} + 6\gamma x$$

$$\Pi(G_1,x) = \sum_c m\cdot c\cdot x^{e-c}$$

$$= 6\sum_{k=1}^{\gamma-1} (\gamma+k)x^{(9\gamma^2+3\gamma)-(\gamma+k)} + 3(2\gamma)x^{(9\gamma^2+3\gamma)-2\gamma} + 6\gamma x^{(9\gamma^2+3\gamma)-1}$$

$$= 6\, x^{9\gamma^2+2\gamma}\left(\frac{\gamma(1-x^{-(\gamma-1)})(x-1)+x\left(1-\gamma x^{-(\gamma-1)}+(\gamma-1)x^{-\gamma}\right)}{(x-1)^2}\right) + 6\gamma\, x^{9\gamma^2+\gamma} + 6\gamma\, x^{9\gamma^2+3\gamma-1}$$

$$Sd(G_1,x) = \sum_c m\cdot\ x^{e-c}$$

$$= 6\sum_{k=1}^{\gamma-1} x^{(9\gamma^2+3\gamma)-(\gamma+k)} + 3x^{(9\gamma^2+3\gamma)-2\gamma} + 6\gamma x^{(9\gamma^2+3\gamma)-1}$$

$$= 6\left(\frac{x^{9\gamma^2+2\gamma}-x^{9\gamma^2+\gamma+1}}{x-1}\right) + 3x^{9\gamma^2+\gamma} + 6\gamma x^{9\gamma^2+3\gamma-1}$$

Corollary 1.1 *Let G_1 Nanographene system with pendant edges of dimension $\gamma = 2$ Then,*

1. $\Omega(G_1,x) = 3x^4 + 6x^3 + 12x$.
2. $\Theta(G_1,x) = 12x^4 + 18x^3 + 12x$.
3. $\Pi(G_1,x) = 12x^{41} + 18x^{39} + 12x^{38}$.
4. $Sd(G_1,x) = 12x^{41} + 6x^{39} + 3x^{38}$.

Proof. The acute edges (A-type) of Nanographene with pendant edges ($\gamma = 2$) is divided into three groups in Figure 5. The three groups are acute edges (A-type)[15] have symmetry about the middle edges (M-type). We therefore count six times in order to determine the counting polynomials in A-type classes. And the middle cuts count 3 times. Then take the pendant edge, each counts as one and the number of times as 12. The graph Graphene and Nano graphene system with pendant edges of dimension $\gamma = 2$, total number of edges is 42.

For the case $\gamma = 2$, the corresponding nanographene structure with pendant edges is shown in Figure 5.

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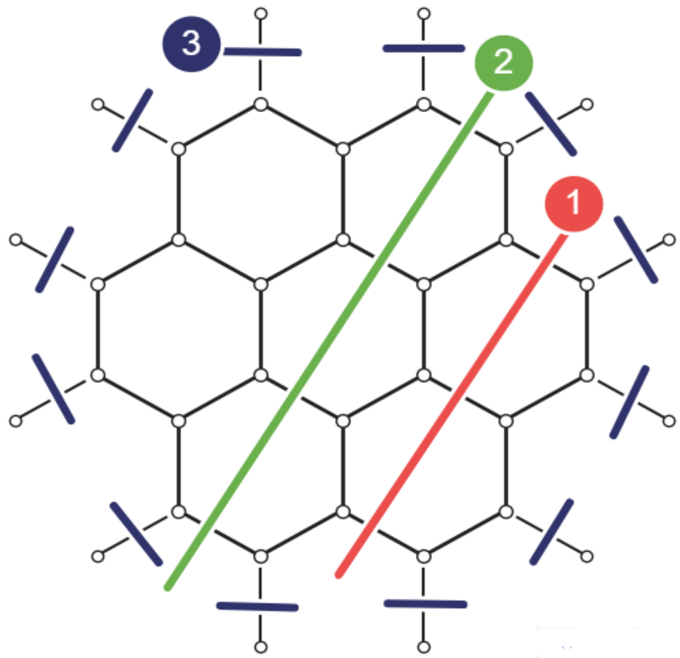

Figure 5: G_1 Nanographene with pendant edges of dimension 2, acute cuts 1, middle cuts 2, and pendant edge cuts 3

From the structure shown in Figure 5, the edge partitions and their corresponding frequencies are listed in Table 2.

Type of Cuts	**Cut cardinality**	**Number of times**
$G_1/_{AC_i}$	3	6
$G_1/_{AM}$	4	3
$G_1/_{PT}$	1	12

Table 2: Edge partitions of Nanographene system with pendant edges of dimension 2.

Using the values given in Table 2 and applying the definition of the Omega polynomial, the required expression is obtained as follows. It is worth noting that the same result can also be obtained directly from Theorem 1 by substituting $\gamma = 2$, which confirms the consistency of the derivation. A similar procedure can be followed to obtain the remaining polynomials.

The Omega polynomial is obtained using the definition

$$\Omega(G, x) = \sum m\, x^c.$$

Using the values from Table 2, we obtain

$$\Omega(G_1, x) = 6x^3 + 3x^4 + 6(2x) = 6x^3 + 3x^4 + 12x.$$

Alternatively, the same result can be obtained from Theorem 1 by substituting $\gamma = 2$:

$$\Omega(G_1, x) = 6\left(\frac{x^{2\gamma} - x^{\gamma+1}}{x-1}\right) + 3x^{2\gamma} + 6\gamma x.$$

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Substituting $\gamma = 2$, we get
$\Omega(G_1, x) = 6x^3 + 3x^4 + 12x.$

In a similar manner, the Theta, Pi, and Sadhana polynomials for $\gamma = 2$ are obtained as
$\Theta(G_1, x) = 12x^4 + 18x^3 + 12x,$
$\Pi(G_1, x) = 12x^{41} + 18x^{39} + 12x^{38},$
$Sd(G_1, x) = 12x^{41} + 6x^{39} + 3x^{38}.$

Theorem 2 *Let G_1 Nanographene system with pendant edges of dimension γ for $\gamma \geq 1$. Then*

1. *Omega index* $\Omega'(G_1, 1) = 9\gamma^2 + 3\gamma = |E(G)|.$
2. *Theta index* $\Theta'(G_1, 1) = 14\gamma^3 - 3\gamma^2 + 7\gamma.$
3. *Pi index* $\Pi'(G_1, 1) = 81\gamma^4 + 40\gamma^3 + 12\gamma^2 - 7\gamma.$
4. *Sadhana index* $Sd'(G_1, 1) = 108\gamma^3 - 12\gamma.$

Proof. Using the counting polynomials obtained in Theorem 1, the corresponding indices are determined by differentiating each polynomial with respect to x and then evaluating the result at $x = 1$.

$$\Omega'(G_1, 1) = \left[\frac{d}{dx}\left(6\left(\frac{x^{2\gamma} - x^{\gamma+1}}{x-1}\right) + 3x^{2\gamma} + 6\gamma x\right)\right]_{x=1}$$

$$= \left[6\left(\frac{(x-1)(2\gamma x^{2\gamma-1} - (\gamma+1)x^{\gamma}) - (x^{2\gamma} - x^{\gamma+1})}{(x-1)^2}\right) + 3(2\gamma)x^{2\gamma-1} + 6\gamma\right]_{x=1}$$

$$= 6\left[\frac{(x-1)(2\gamma x^{2\gamma-1} - (\gamma+1)x^{\gamma}) - (x^{2\gamma} - x^{\gamma+1})}{(x-1)^2}\right]_{x=1} + 12\gamma$$

$$= 6\left[\frac{0}{0}\right] + 12\gamma.$$

Applying L hospitals rule

$$= 6\left[\frac{\frac{d}{dx}\left((x-1)(2\gamma x^{2\gamma-1} - (\gamma+1)x^{\gamma}) - (x^{2\gamma} - x^{\gamma+1})\right)}{\frac{d}{dx}(x-1)^2}\right]_{x=1} + 12\gamma$$

$$= 6\left[\frac{(2\gamma x^{2\gamma-1} - (\gamma+1)x^{\gamma}) + (x-1)(2\gamma(2\gamma-1)x^{2\gamma-2} - \gamma(\gamma+1)x^{\gamma-1}) - (2\gamma x^{2\gamma-1} - (\gamma+1)x^{\gamma})}{2(x-1)}\right]_{x=1} + 12\gamma$$

$$= 6\left[\frac{(x-1)(2\gamma(2\gamma-1)x^{2\gamma-2} - \gamma(\gamma+1)x^{\gamma-1})}{2(x-1)}\right]_{x=1} + 12\gamma$$

$$= 6\left[\frac{2\gamma(2\gamma-1)x^{2\gamma-2} - \gamma(\gamma+1)x^{\gamma-1}}{2}\right]_{x=1} + 12\gamma$$

$$= 6\left[\frac{2\gamma(2\gamma-1) - \gamma(\gamma+1)}{2}\right] + 12\gamma$$

$$= 6\left[\frac{4\gamma^2 - 2\gamma - \gamma^2 - \gamma}{2}\right] + 12\gamma$$

$$= 6\left[\frac{3\gamma^2 - 3\gamma}{2}\right] + 12\gamma$$

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$$= 9\gamma^2 - 9\gamma + 12\gamma$$
$$= 9\gamma^2 + 3\gamma = |E(G)|.$$

$$\Theta'(G_1,1) = [\frac{d}{dx}\left(6\left(\frac{\gamma x^{\gamma+1}(x^{\gamma-1}-1)}{x-1} + \frac{x^{\gamma+1}(1-\gamma x^{\gamma-1}+(\gamma-1)x^{\gamma})}{(x-1)^2}\right) + 6\gamma x^{2\gamma} + 6\gamma x\right)]_{x=1}$$
$$= [6\left(\frac{(x-1)(\gamma(\gamma+1)x^{\gamma}-2\gamma^2 x^{2\gamma-1}) - \gamma(x^{\gamma+1}-x^{2\gamma})}{(x-1)^2}\right)$$
$$+6\left(\frac{(x-1)^2(\gamma+1)x^{\gamma}-2\gamma^2x^{2\gamma-1}+(\gamma-1)(2\gamma+1)x^{2\gamma}-(x^{\gamma+1}-\gamma x^{2\gamma}+(\gamma-1)x^{2\gamma+1})(-2)(x-1)}{(x-1)^4}\right)$$
$$+6\gamma(2\gamma)x^{2\gamma-1} + 6\gamma]_{x=1}$$
$$= \frac{0}{0}.$$

Applying L hospitals rule

$$\Theta'(G_1,1) = 14\gamma^3 - 3\gamma^2 + 7\gamma.$$

$$\Pi'(G_1,1) = \frac{d}{dx}[6\, x^{9\gamma^2+2\gamma}\left(\frac{\gamma(1-x^{-(\gamma-1)})(x-1) + x(1-\gamma x^{-(\gamma-1)} + (\gamma-1)x^{-\gamma})}{(x-1)^2}\right)$$
$$+ 6\gamma\, x^{9\gamma^2+\gamma} + 6\gamma\, x^{9\gamma^2+3\gamma-1}]_{x=1}$$
$$= [6\left((9\gamma^2+2\gamma)x^{9\gamma^2+2\gamma-1}[\gamma(1-x^{-(\gamma-1)})(x-1) + x(1-\gamma x^{-(\gamma-1)} + (\gamma-1)x^{-\gamma})]\right)/(x-1)^2$$
$$+6\left(\frac{x^{9\gamma^2+2\gamma}[2\gamma(\gamma-1)x^{-\gamma}(x-1)+2-2\gamma x^{-(\gamma-1)}+(\gamma-1)x^{-\gamma}](x-1)}{(x-1)^3}\right)$$
$$-12\left(\frac{[\gamma(1-x^{-(\gamma-1)})(x-1)+x(1-\gamma x^{-(\gamma-1)}+(\gamma-1)x^{-\gamma})]}{(x-1)^3}\right)]_{x=1}$$
$$= \frac{0}{0}.$$

Applying L hospitals rule

$$\Pi'(G_1,1) = 81\gamma^4 + 40\gamma^3 + 12\gamma^2 - 7\gamma.$$

$$Sd'(G_1,1) = [\frac{d}{dx}\left(6\left(\frac{x^{9\gamma^2+2\gamma} - x^{9\gamma^2+\gamma+1}}{x-1}\right) + 3x^{9\gamma^2+\gamma} + 6\gamma x^{9\gamma^2+3\gamma-1}\right)]_{x=1}$$
$$= [6\,\frac{(9\gamma^2+2\gamma)x^{9\gamma^2+2\gamma-1} - (9\gamma^2+\gamma+1)x^{9\gamma^2+\gamma}(x-1) - (x^{9\gamma^2+2\gamma} - x^{9\gamma^2+\gamma+1})}{(x-1)^2}$$
$$+3(9\gamma^2+\gamma) + 6\gamma(9\gamma^2+3\gamma-1)x^{9\gamma^2+3\gamma-1}]_{x=1}$$
$$= \frac{0}{0}.$$

Applying L hospitals rule

$$Sd'(G_1,1) = 108\gamma^3 - 12\gamma.$$

Corollary 2.1

Let G_1 Nanographene system with pendant edges of dimension $\gamma = 2$. Then,

1. *Omega index $\Omega'(G_1,1) = 42 = |E(G)|$.*
2. *Theta index $\Theta'(G_1,1) = 18$.*
3. *Pi index $\Pi'(G_1,1) = 126$.*
4. *Sadhana index $Sd'(G_1,1) = 96$.*

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Proof. Using the counting polynomials obtained in Corollary 1.1, we compute the corresponding indices as follows:

$$\Omega'(G_1, 1) = \left[\frac{d}{dx}(3x^4 + 6x^3 + 12x)\right]_{x=1}$$
$$= 42.$$

Alternatively, by substituting $\gamma = 2$ in the general result in theorem 2, we obtain

$$\Omega'(G_1, 1) = 9\gamma^2 + 3\gamma$$
$$= 9(2)^2 + 3(2)$$
$$= 42.$$

Similarly, the remaining indices are obtained as

$$\Theta'(G_1, 1) = 18,$$
$$\Pi'(G_1, 1) = 126,$$
$$Sd'(G_1, 1) = 96.$$

In order to illustrate the applicability of the derived results, the numerical values of the corresponding topological indices are computed for different values of the dimension. The computed values are presented in Table 3.

Table 3: Computed values of topological indices for $\gamma = 1$ to 10

γ	$\Omega'(G_1, 1)$	$\Theta'(G_1, 1)$	$\Pi'(G_1, 1)$	$Sd'(G_1, 1)$
1	12	18	126	96
2	42	114	1650	840
3	90	372	7728	2880
4	156	876	23460	6864
5	240	1710	55890	13440
6	342	2958	114006	23256
7	462	4704	208740	36960
8	600	7032	352968	55200
9	756	10026	561510	78624
10	930	13770	851130	107880

From Table 3, it is observed that all the considered indices increase as the dimension γ increases. In particular, the growth of the Pi index is significantly higher compared to the other indices, indicating its stronger dependence on the size of the structure.

To better understand the variation of these indices with respect to γ, a graphical representation is provided in Figure 6.

https://doi.org/10.71058/jodac.v10i04020

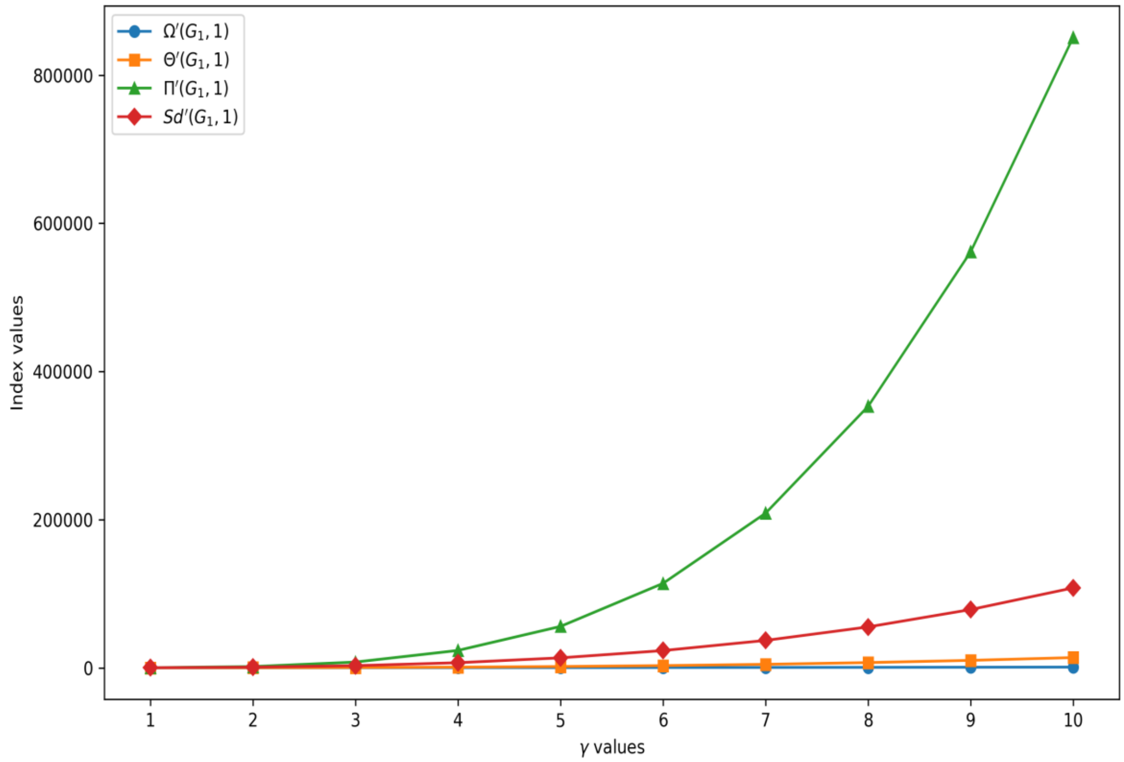

Figure 6: Graphical representation of topological indices with respect to γ.

The graphical representation indicates that all the considered indices increase as the dimension γ increases. It can be observed that the Pi index grows at a significantly faster rate compared to the Omega, Theta, and Sadhana indices, which show a more gradual increase. This behavior suggests that triangular nanographene with pendant edges is highly sensitive to structural expansion. Such a trend may offer useful insights into the structural properties of these nanographene systems, and it motivates further investigation to better understand this behavior in more complex configurations.

Theorem 3 *Let G_2 be a Triangle-shaped Graphene system with pendant edges of dimension γ for $\gamma \geq 1$, Then,*

1. $\Omega(G_2,x) = 3\left(\frac{x^{\gamma+2}-1}{x-1}\right) + 3\gamma x - 3$

2. $\Theta(G_2,x) = 3\left(\frac{2x^2-x^3-(\gamma+2)x^{\gamma+2}+(\gamma+1)x^{\gamma+3}}{(x-1)^2}\right) + (3\gamma+3)x$

3. $\Pi(G_2,x) = 3\frac{x^{\frac{3\gamma^2+15\gamma+6}{2}}}{(x-1)^2}\left(2-\frac{1}{x}-(\gamma+2)\frac{1}{x^{\gamma}}+(\gamma+1)\frac{1}{x^{\gamma+1}}\right) + (3\gamma+3)x^{\frac{3\gamma^2+15\gamma+4}{2}}$

4. $Sd(G_2,x) = 3\left(\frac{x^{\frac{3\gamma^2+15\gamma+4}{2}}-x^{\frac{3\gamma^2+13\gamma+4}{2}}}{x-1}\right) + (3\gamma+3)x^{\frac{3\gamma^2+15\gamma+4}{2}}$

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Proof. The acute edges (A-type) of Triangle shaped with Graphene and Nanographene with pendant edges ($\gamma = 4$) is divided into two groups in in Figure 4. We therefore count three times in order to determine the counting polynomials in A-type classes[12, 13, 17, 18]. Then take the pendant edge, each counts as one and the number of times as $3\gamma + 3$. As a result, we can find the counting polynomial equations from the graph theoritical parameters shown in Table 2. The Triangle shaped graph Graphene and Nano graphene system with pendant edges of dimension γ, total number of edges is $\frac{3\gamma^2+15\gamma+6}{2}$.

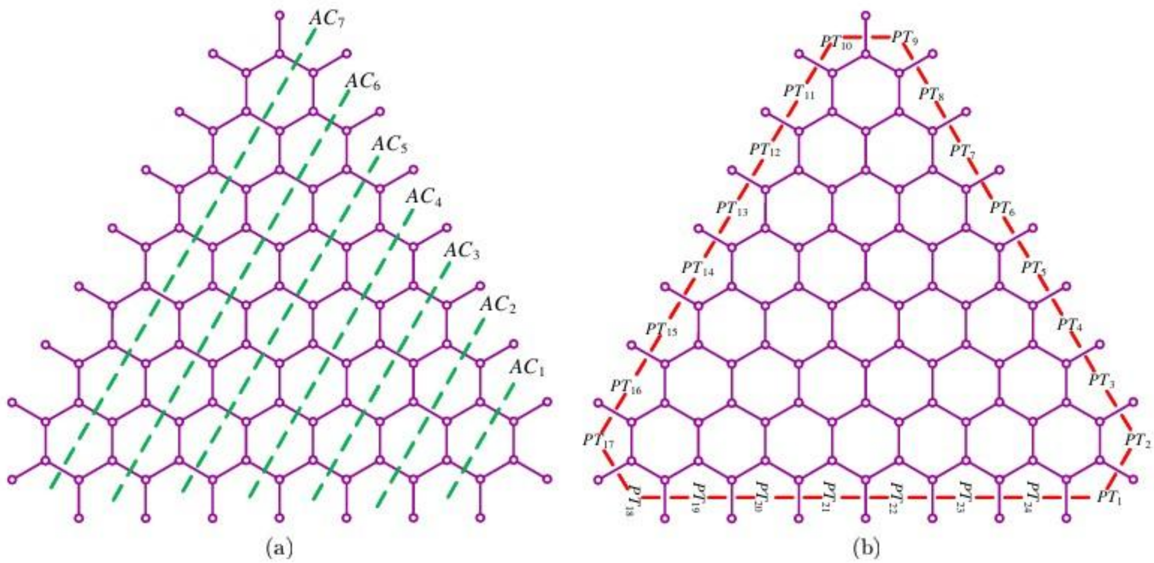

Figure 7: G_2 Triangle shaped Nanographene system with pendant edges of dimension 4 (a)G_2 acute cuts, Ranges $1 \leq i \leq \gamma$; (b)G_2 Pendant edge cuts, Ranges $1 \leq i \leq 3\gamma + 3$.

From the structure shown in Figure 7, the edge partitions and their corresponding frequencies are listed in Table 4.

Type of Cuts	Ranges	Number of edge cuts	Number of times
$G_2/_{AC_i}$	$1 \leq i \leq \gamma$	$i + 1$	3
$G_2/_{PT_i}$	$1 \leq i \leq 3\gamma + 3$	1	1

Table 4: Edge partitions of triangle shaped Nanographene system with pendant edges of dimension 4.

Using the values given in Table 4 and applying the definition of Omega(Ω), Theta(θ), Pi(π), and Sadhana(Sd) polynomials, the required expression is obtained as follows.

$$\Omega(G_2, x) = 3\sum_{k=1}^{\gamma} x^{k+1} + (3\gamma + 3)x$$
$$= 3\left(\frac{x^{\gamma+2}-1}{x-1}\right) + 3\gamma x - 3$$

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$$\Theta(G_2,x) = 3\sum_{k=1}^{\gamma}(k+1)x^{k+1} + (3\gamma+3)x$$
$$= 3\left(\frac{2x^2 - x^3 - (\gamma+2)x^{\gamma+2} + (\gamma+1)x^{\gamma+3}}{(1-x)^2}\right) + (3\gamma+3)x$$
$$\Pi(G_2,x) = 3\sum_{k=1}^{\gamma}(k+1)x^{\frac{3\gamma^2+15\gamma+6}{2}-(k+1)} + (3\gamma+3)x^{\frac{3\gamma^2+15\gamma+6}{2}-1}$$
$$= 3\,\frac{x^{\frac{3\gamma^2+15\gamma+6}{2}}}{(x-1)^2}\left(2 - \frac{1}{x} - (\gamma+2)\frac{1}{x^{\gamma}} + (\gamma+1)\frac{1}{x^{\gamma+1}}\right) + (3\gamma+3)x^{\frac{3\gamma^2+15\gamma+4}{2}}$$
$$Sd(G_2,x) = 3\sum_{k=1}^{\gamma}x^{\frac{3\gamma^2+15\gamma+6}{2}-(k+1)} + (3\gamma+3)x^{\frac{3\gamma^2+15\gamma+6}{2}-1}$$
$$= 3\left(\frac{x^{\frac{3\gamma^2+15\gamma+4}{2}} - x^{\frac{3\gamma^2+13\gamma+4}{2}}}{x-1}\right) + (3\gamma+3)x^{\frac{3\gamma^2+15\gamma+4}{2}}$$

Corollary 3.1 *Let G_2 Triangle-shaped Graphene system with pendant edges of dimension $\gamma = 2$ Then,*

1. $\Omega(G_2,x) = 3x^3 + 3x^2 + 9x$
2. $\Theta(G_2,x) = 9x^3 + 6x^2 + 9x$
3. $\Pi(G_2,x) = 9x^{23} + 6x^{22} + 9x^{21}$
4. $Sd(G_2,x) = 9x^{23} + 3x^{22} + 3x^{21}$.

Proof. The acute edges (A-type) of Nanographene with pendant edges ($\gamma = 2$) is divided into three groups in Figure 8. The three groups are acute edges (A-type)[15] have symmetry about the middle edges (M-type). We therefore count six times in order to determine the counting polynomials in A-type classes. And the middle cuts count 3 times. Then take the pendant edge, each counts as one and the number of times as 12. As a result, we can find the counting polynomial equations from the graph theoritical parameters shown in Table 2. The Triangular nano graphene system with pendant edges of dimension $\gamma = 2$, total number of edges is 24.

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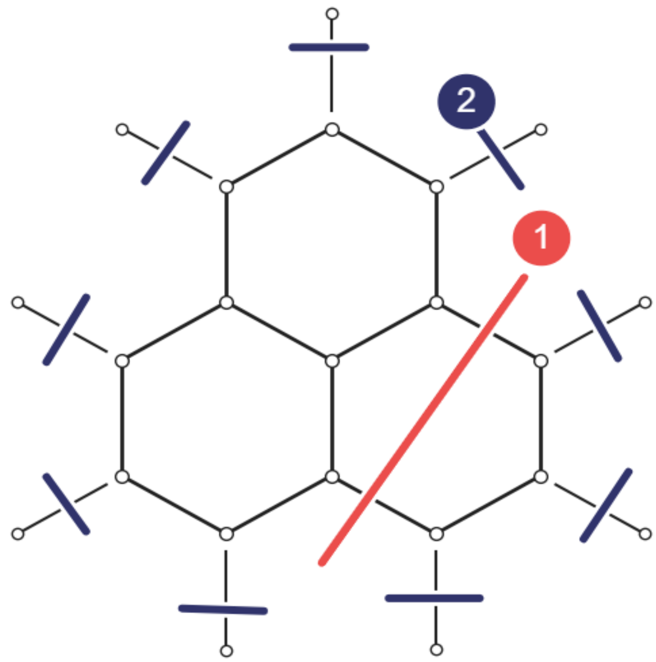

Figure 8: G_1 Nanographene system with pendant edges of dimension 4 (a) G_1 acute cuts (1) , Ranges $1 \leq i \leq 2$ and G_1 pendant edge cuts (2)

Type of Cuts	Ranges	Number of edge cuts	Number of times
$G_2/_{AC_i}$	$1 \leq i \leq 2$	$i+1$	3
$G_2/_{PT_i}$	1	1	9

Table 5: Edge partitions of triangle shaped Nanographene system with pendant edges of dimension 4.

Using the values given in Table 5 and applying the definition of the Omega polynomial, the required expression is obtained as follows. It is worth noting that the same result can also be obtained directly from Theorem 3 by substituting $\gamma = 2$, which confirms the consistency of the derivation. A similar procedure can be followed to obtain the remaining polynomials.

The Omega polynomial is obtained using the definition

$\Omega(G,x) = \sum m\, x^c$.

Using the values from Table 2, we obtain

$\Omega(G_2,x) = 3x^2 + 3x^3 + 9(1x) = 3x^3 + 3x^2 + 9x$.

Alternatively, the same result can be obtained from Theorem 3

$\Omega(G_2,x) = 3\left(\frac{x^{\gamma+2}-1}{x-1}\right) + 3\gamma x - 3$.

Substituting $\gamma = 2$, we obtain

$\Omega(G_2,x) = 3\left(\frac{x^{4}-1}{x-1}\right) + 6x - 3$.

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Using the identity $\frac{x^4-1}{x-1}=1+x+x^2+x^3$ we get
$\Omega(G_2,x)=3+3x+3x^2+3x^3+6x-3=3x^3+3x^2+9x.$

In a similar manner, the Theta, Pi, and Sadhana polynomials for $\gamma=2$ are obtained as
$\Theta(G_2,x)=9x^3+6x^2+9x$
$\Pi(G_2,x)=9x^{23}+6x^{22}+9x^{21}$
$Sd(G_2,x)=9x^{23}+3x^{22}+3x^{21}.$

Theorem 4 *Let G_2 be a Triangle-shaped Graphene system with pendant edges of dimension γ for $\gamma\geq 1$, Then,*

1. $\Omega'(G_2,1)=\frac{3\gamma^2+15\gamma+6}{2}=|E(G)|.$
2. $\Theta'(G_2,1)=\frac{2\gamma^3+9\gamma^2+19\gamma+6}{2}.$
3. $\Pi'(G_2,1)=\frac{9\gamma^4+86\gamma^3+243\gamma^2+142\gamma+24}{4}.$
4. $Sd'(G_2,1)=9\gamma^3+48\gamma^2+33\gamma+6.$

Proof. Using the counting polynomials obtained in Theorem 3, the corresponding indices are determined by differentiating each polynomial with respect to x and then evaluating the result at $x=1$.

$$\Omega'(G_2,1)=\left[\frac{d}{dx}\left(3\left(\frac{x^{\gamma+2}-1}{x-1}\right)+3\gamma x-3\right)\right]_{x=1}$$
$$=\left[3\left(\frac{(x-1)\left((\gamma+2)x^{\gamma+1}\right)-\left(x^{\gamma+2}-1\right)}{(x-1)^2}\right)+3\gamma\right]_{x=1}$$
$$=3\left[\frac{(x-1)\left((\gamma+2)x^{\gamma+1}\right)-\left(x^{\gamma+2}-1\right)}{(x-1)^2}\right]_{x=1}+3\gamma$$
$$=3\left[\frac{0}{0}\right]+3\gamma.$$

Applying L hospitals rule

$$=3\left[\frac{\frac{d}{dx}\left((x-1)\left((\gamma+2)x^{\gamma+1}\right)-\left(x^{\gamma+2}-1\right)\right)}{\frac{d}{dx}(x-1)^2}\right]_{x=1}+3\gamma$$
$$=3\left[\frac{(\gamma+2)x^{\gamma+1}+(x-1)(\gamma+2)(\gamma+1)x^{\gamma}-(\gamma+2)x^{\gamma+1}}{2(x-1)}\right]_{x=1}+3\gamma$$
$$=3\left[\frac{(x-1)(\gamma+2)(\gamma+1)x^{\gamma}}{2(x-1)}\right]_{x=1}+3\gamma$$
$$=3\left[\frac{(\gamma+2)(\gamma+1)x^{\gamma}}{2}\right]_{x=1}+3\gamma$$
$$=3\left[\frac{(\gamma+2)(\gamma+1)}{2}\right]+3\gamma$$
$$=\frac{3\left(\gamma^2+3\gamma+2\right)}{2}+3\gamma$$

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$= \frac{3\gamma^2+9\gamma+6+6\gamma}{2}$
$= \frac{3\gamma^2+15\gamma+6}{2}$
$= |E(G)|.$

$$\Theta'(G_2,x) = [\frac{d}{dx}\left(3\left(\frac{2x^2-x^3-(\gamma+2)x^{\gamma+2}+(\gamma+1)x^{\gamma+3}}{(x-1)^2}\right) + (3\gamma+3)x\right)]_{x=1}$$
$$= [\frac{3(x-1)[4x-3x^2-(\gamma+2)^2x^{\gamma+1}+(\gamma+1)(\gamma+3)x^{\gamma+2}]}{(x-1)^4} - \frac{6(x-1)[2x^2-x^3-(\gamma+2)x^{\gamma+2}+(\gamma+1)x^{\gamma+3}]}{(x-1)^4} + (3\gamma+3)]_{x=1}$$
$$= \frac{0}{0}$$

Applying L hospitals rule

$\Theta'(G_2,1) = \frac{2\gamma^3+9\gamma^2+19\gamma+6}{2}$

$$\Pi'(G_2,1) = \left[\frac{d}{dx}\left(3\frac{x^{\frac{3\gamma^2+15\gamma+6}{2}}}{(x-1)^2}\left(2-\frac{1}{x}-(\gamma+2)\frac{1}{x^\gamma}+(\gamma+1)\frac{1}{x^{\gamma+1}}\right) + (3\gamma+3)x^{\frac{3\gamma^2+15\gamma+4}{2}}\right)\right]_{x=1}.$$
$$= \frac{9\gamma^4+86\gamma^3+243\gamma^2+142\gamma+24}{4}.$$

$$Sd'(G_2,1) = \left[\frac{d}{dx}\left(3\left(\frac{x^{\frac{3\gamma^2+15\gamma+4}{2}} - x^{\frac{3\gamma^2+13\gamma+4}{2}}}{x-1}\right) + (3\gamma+3)x^{\frac{3\gamma^2+15\gamma+4}{2}}\right)\right]_{x=1}.$$
$$= 9\gamma^3+48\gamma^2+33\gamma+6.$$

Corollary 4.1

Let G_2 be a Triangle-shaped Graphene system with pendant edges of dimension $\gamma = 2$, Then

1. $\Omega'(G_2,1) = 24 = |E(G)|.$
2. $\Theta'(G_2,1) = 42.$
3. $\Pi'(G_2,1) = 198.$
4. $Sd'(G_2,1) = 216.$

Proof. Using the counting polynomials obtained in Corollary 3.1, we compute the corresponding indices as follows:

$$\Omega'(G_2,1) = \left[\frac{d}{dx}(3x^3+3x^2+9x)\right]_{x=1}$$
$$= (9x^2+6x+9)_{x=1}$$
$$= 9(1)^2+6(1)+9$$
$$= 9+6+9$$

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$= 24.$

Alternatively, substituting the dimension $\gamma = 2$ in the general result in theorem 4, we get $\Omega'(G_2, 1) = \frac{3\gamma^2+15\gamma+6}{2} = 24$. Similarly the remaining indices are obtained as

$\Theta'(G_2, 1) = 42,$
$\Pi'(G_2, 1) = 198,$
$Sd'(G_2, 1) = 216.$

In order to illustrate the applicability of the derived results, the numerical values of the corresponding topological indices are computed for different values of the dimension. The computed values are presented in Table 6.

Table 6: Computed values of topological indices for $\gamma = 1$ to 10

γ	$\Omega'(G_2, 1)$	$\Theta'(G_2, 1)$	$\Pi'(G_2, 1)$	$Sd'(G_2, 1)$
1	12	18	126	96
2	24	48	528	336
3	39	99	1422	780
4	57	177	3072	1482
5	78	288	5796	2496
6	102	438	9966	3876
7	129	633	16008	5676
8	159	879	24402	7950
9	192	1182	35682	10752
10	228	1548	50436	14136

From Table 6, it is observed that all the considered indices increase as the dimension γ increases. In particular, the growth of the Pi index is significantly higher compared to the other indices, indicating its stronger dependence on the size of the structure.

To better understand the variation of these indices with respect to γ, a graphical representation is provided in Figure 9.

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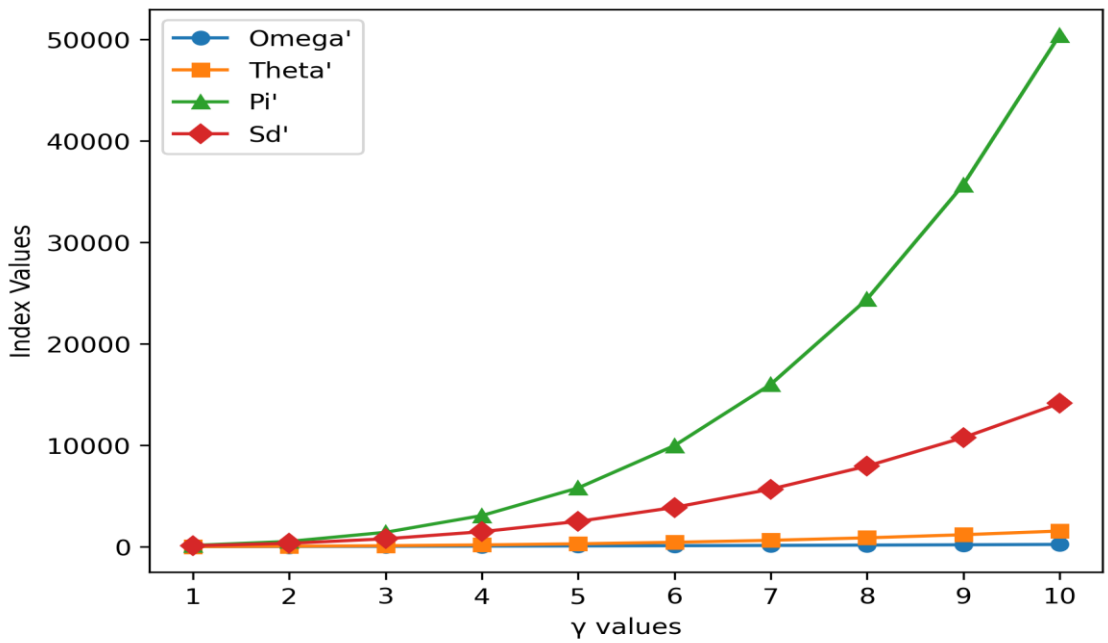

Figure 9: Graphical representation of topological indices with respect to γ.

The graphical representation indicates that all the considered indices increase as the dimension γ increases. It can be observed that the Pi index grows at a significantly faster rate compared to the Omega, Theta, and Sadhana indices, which show a more gradual increase. This behavior suggests that triangular nanographene with pendant edges is highly sensitive to structural expansion. Such a trend may offer useful insights into the structural properties of these nanographene systems, and it motivates further investigation to better understand this behavior in more complex configurations.

6. Graph Construction, Construct Counting Polynomials, and the Corresponding Indices of Nanographene with Pendant Edges: A Python-Based Approach

In this section, we present a Python implementation for constructing Nanographene e structure with pendant edges and computing the associated four specific polynomials namely, the Omega(Ω), Theta(θ), Pi(π), and Sadhana(Sd) polynomials , and the subsequent indices are obtained for both classes of structures. Using the derived theoretical expressions, the implementation enables efficient generation of structures and rapid evaluation of the polynomials and indices for arbitrary dimension γ.

```
import math
import matplotlib.pyplot as plt
from collections import defaultdict

poly_val = lambda g: {
    "Omega'": (3 * g**2 + 15 * g + 6) / 2,
```

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```
    "Theta'": (2 * g**3 + 9 * g**2 + 19 * g + 6) / 2,
    "Pi'": (9 * g**4 + 86 * g**3 + 243 * g**2 + 142 * g + 24) / 4,
    "Sd'": 9 * g**3 + 48 * g**2 + 33 * g + 6
}

clean = lambda p: {k: v for k, v in p.items() if abs(v) > 1e-9}


def E1(t):
    c = {}
    if t >= 2:
        for k in range(t + 1, 2 * t):
            c[k] = c.get(k, 0) + 6
    if t == 0:
        c[0] = -6
    c[2 * t] = c.get(2 * t, 0) + 3
    if t:
        c[1] = c.get(1, 0) + 6 * t
    return clean(c)


def div(N):
    den = {0: 1, 1: -2, 2: 1}
    res = {}
    N = dict(N)

    while N and max(N) >= 2:
        d = max(N)
        f = N[d]
        s = d - 2
        res[s] = res.get(s, 0) + f

        for k, v in den.items():
            key = k + s
            N[key] = N.get(key, 0) - f * v
            if abs(N[key]) < 1e-9:
                N.pop(key)

    return res


def E2(t):
    c = {}
    if t >= 2:
        for k in range(t + 1, 2 * t):
            c[k] = c.get(k, 0) + 6 * t
```

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```
    for d, v in div({t + 1: 1, 2 * t: -t, 2 * t + 1: t - 1}).items():
        c[d] = c.get(d, 0) + 6 * v

    c[2 * t] = c.get(2 * t, 0) + 6 * t
    if t:
        c[1] = c.get(1, 0) + 6 * t
    return clean(c)


def E3(t):
    c = {}
    S = 9 * t * t

    for d, v in div({t + 1: t + 1, t: -t, 2: -2 * t, 1: 2 * t - 1}).items():
        c[d + S + t] = c.get(d + S + t, 0) + 6 * v

    c[S + t] = c.get(S + t, 0) + 6 * t

    if t >= 1:
        c[S + 3 * t - 1] = c.get(S + 3 * t - 1, 0) + 6 * t

    return clean(c)


def E4(t):
    c = {}
    S = 9 * t * t
    A, B = S + 2 * t, S + t + 1

    if A > B:
        for k in range(B, A):
            c[k] = c.get(k, 0) + 6

    c[S + t] = c.get(S + t, 0) + 3

    if t >= 1:
        c[S + 3 * t - 1] = c.get(S + 3 * t - 1, 0) + 6 * t

    return clean(c)


def fmt(p):
    if not p:
        return "0"
```

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```
    s = ""
    for d in sorted(p, reverse=True):
        c = p[d]
        coeff = "" if abs(c) == 1 and d else str(int(abs(c)))
        var = "x" if d else ""
        power = "^" + str(d) if d > 1 else ""
        term = f"{coeff}{var}{power}"

        if not s:
            s = ("-" if c < 0 else "") + term
        else:
            s += (" - " if c < 0 else " + ") + term

    return s


def draw(g):
    s = 1
    color = "#222222"

    C = [
        (s * 3**0.5 * (q + r / 2), 1.5 * s * r)
        for q in range(-g, g + 1)
        for r in range(max(-g, -q - g), min(g, -q + g) + 1)
    ]

    H = [
        [
            (
                x + s * math.cos(math.radians(60 * i + 30)),
                y + s * math.sin(math.radians(60 * i + 30))
            )
            for i in range(6)
        ]
        for x, y in C
    ]

    E = {}
    V = defaultdict(int)

    for h in H:
        for i in range(6):
            p1 = tuple(round(x, 6) for x in h[i])
            p2 = tuple(round(x, 6) for x in h[(i + 1) % 6])
            k = tuple(sorted((p1, p2)))
            E[k] = E.get(k, 0) + 1
```

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```
        V[p1] += 1

    cx = sum(x for x, _ in C) / len(C)
    cy = sum(y for _, y in C) / len(C)

    N = defaultdict(list)
    for (p1, p2), c in E.items():
        if c == 1:
            ex, ey = p2[0] - p1[0], p2[1] - p1[1]
            for nx, ny in [(ey, -ex), (-ey, ex)]:
                if ((p1[0] + p2[0]) / 2 - cx) * nx + ((p1[1] + p2[1]) / 2 - cy) * ny >= 0:
                    l = (nx**2 + ny**2) ** 0.5
                    nx, ny = nx / l, ny / l
                    N[p1].append((nx, ny))
                    N[p2].append((nx, ny))
                    break

    fig, ax = plt.subplots(figsize=(10, 7))

    for (p1, p2) in E:
        ax.plot([p1[0], p2[0]], [p1[1], p2[1]], lw=2, color=color, zorder=1)

    for v, n in N.items():
        if V[v] == 1:
            nx = sum(i[0] for i in n) / len(n)
            ny = sum(i[1] for i in n) / len(n)
            l = (nx**2 + ny**2) ** 0.5
            nx, ny = nx / l, ny / l
            hx, hy = v[0] + nx * s, v[1] + ny * s
            sx, sy = v[0] + nx * 0.15, v[1] + ny * 0.15
            ax.plot([sx, hx], [sy, hy], lw=1.5, color=color, zorder=1)

    for v in V:
        ax.plot(v[0], v[1], 'o', ms=7, mfc='white', mec=color, linewidth=1.5, zorder=3)

    for v, n in N.items():
        if V[v] == 1:
            nx = sum(i[0] for i in n) / len(n)
            ny = sum(i[1] for i in n) / len(n)
            l = (nx**2 + ny**2) ** 0.5
            nx, ny = nx / l, ny / l
            hx, hy = v[0] + nx * s, v[1] + ny * s
            ax.plot(hx, hy, 'o', ms=6, mfc='white', mec=color, zorder=3)

    ax.set_aspect('equal')
    ax.axis('off')
```

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```
    plt.subplots_adjust(right=0.65)

    t = g + 1
    val = poly_val(t)

    k1, k2, k3, k4 = "Omega'", "Theta'", "Pi'", "Sd'"

    f = lambda x: f"{int(x)}" if abs(x - int(x)) < 1e-9 else f"{x:.2f}"

    top = (
        f"Polynomial Equations:\n\n"
        f"Omega(G1,x) = {fmt(E1(t))}\n\n"
        f"Theta(G1,x) = {fmt(E2(t))}\n\n"
        f"Pi(G1,x) = {fmt(E3(t))}\n\n"
        f"Sd(G1,x) = {fmt(E4(t))}"
    )

    bottom = (
        f"Index Values:\n\n"
        f"Omega' = {f(val[k1])}\n\n"
        f"Theta' = {f(val[k2])}\n\n"
        f"Pi' = {f(val[k3])}\n\n"
        f"Sd' = {f(val[k4])}"
    )

    fig.text(0.7, 0.88, top, fontsize=9, bbox=dict(boxstyle="round", fc="white"))
    fig.text(0.7, 0.25, bottom, fontsize=10, bbox=dict(boxstyle="round", fc="white"))

    ax.set_title(f"Nanographene (gamma = {t})")
    plt.show()


draw(int(input("Enter gamma: ")) - 1)
```

7 Sample Output for Nanographene with Pendant Edges)

The above Python implementation is executed for the dimension $\gamma = 5$ to generate the corresponding graph structure and compute the associated counting polynomials and topological indices. The results are obtained within a computational time of five seconds, demonstrating the efficiency of the proposed approach. The sample output obtained from the program is presented below.

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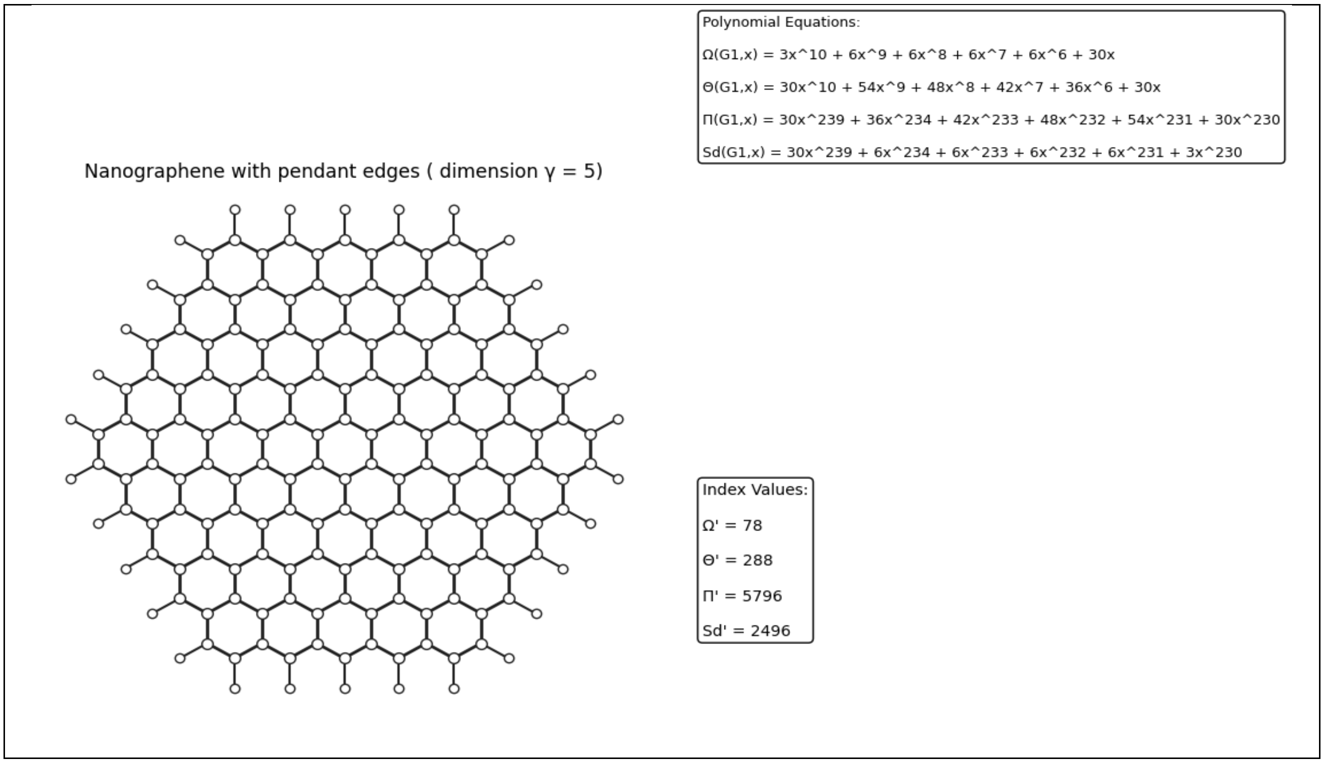

Figure 10: Python-based visualization and verification of the nanographene structure, counting polynomials, and corresponding indices for dimension $\gamma = 5$.

The computed results are consistent with the theoretical values derived in the previous section, thereby validating the correctness of the proposed approach.

8 Graph Construction, Construct Counting Polynomials, and the Corresponding Indices of Triangular Nanographene with Pendant Edges: A Python-Based Approach

In this section, we present a Python implementation for constructing Triangular Nanographene structure with pendant edges and computing the associated four specific polynomials namely, the Omega(Ω), Theta(θ), Pi(π), and Sadhana(Sd) polynomials , and the subsequent indices are obtained for both classes of structures. Using the derived theoretical expressions, the implementation enables efficient generation of structures and rapid evaluation of the polynomials and indices for arbitrary dimension γ.

```
import math
import matplotlib.pyplot as plt
from collections import defaultdict

# ---------- Polynomial Values ----------
poly_val = lambda g: {
    "Omega'": (3*g**2 + 15*g + 6)/2,
```

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```
    "Theta'": (2*g**3 + 9*g**2 + 19*g + 6)/2,
    "Pi'": (9*g**4 + 86*g**3 + 243*g**2 + 142*g + 24)/4,
    "Sd'": 9*g**3 + 48*g**2 + 33*g + 6
}

clean = lambda p: {k: v for k, v in p.items() if abs(v) > 1e-9}


# ---------- Polynomial Formatting ----------
def fmt(p):
    if not p:
        return "0"

    s = ""
    for d in sorted(p, reverse=True):
        c = p[d]
        coeff = "" if abs(c) == 1 and d else str(int(abs(c)))
        var = "x" if d else ""
        power = "^" + str(d) if d > 1 else ""
        term = f"{coeff}{var}{power}"

        if not s:
            s = "-" + term if c < 0 else term
        else:
            s += (" - " if c < 0 else " + ") + term

    return s


# ---------- Simple Polynomial Placeholders ----------
def E1(t):
    return {2*t: 3, 1: 6*t}

def E2(t):
    return {2*t: 6*t, 1: 6*t}

def E3(t):
    return {3*t: 6*t}

def E4(t):
    return {2*t: 3}


# ---------- DRAW FUNCTION ----------
def draw(g):
    s = 1
```

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```
C = [
    (s * 3**0.5 * (q + r/2), 1.5 * s * r)
    for q in range(g + 1)
    for r in range(g + 1 - q)
]

H = [
    [
        (
            x + s * math.cos(math.radians(60*i + 30)),
            y + s * math.sin(math.radians(60*i + 30))
        )
        for i in range(6)
    ]
    for x, y in C
]

E = {}
V = defaultdict(int)

for h in H:
    for i in range(6):
        p1 = tuple(round(x, 6) for x in h[i])
        p2 = tuple(round(x, 6) for x in h[(i + 1) % 6])
        k = tuple(sorted((p1, p2)))
        E[k] = E.get(k, 0) + 1
        V[p1] += 1

cx = sum(x for x, _ in C) / len(C)
cy = sum(y for _, y in C) / len(C)

N = defaultdict(list)

for (p1, p2), c in E.items():
    if c == 1:
        ex, ey = p2[0] - p1[0], p2[1] - p1[1]
        for nx, ny in [(ey, -ex), (-ey, ex)]:
            if ((p1[0] + p2[0]) / 2 - cx) * nx + ((p1[1] + p2[1]) / 2 - cy) * ny >= 0:
                l = (nx**2 + ny**2)**0.5
                nx, ny = nx / l, ny / l
                N[p1].append((nx, ny))
                N[p2].append((nx, ny))
                break

fig, ax = plt.subplots(figsize=(12, 7))
```

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```
plt.subplots_adjust(right=0.6)

for (p1, p2) in E:
    ax.plot([p1[0], p2[0]], [p1[1], p2[1]], lw=2, color='black')

for v in V:
    ax.plot(v[0], v[1], 'o', ms=6, mfc='white', mec='black')

ax.set_aspect('equal')
ax.axis('off')

for v, n in N.items():
    if V[v] == 1:
        nx = sum(i[0] for i in n) / len(n)
        ny = sum(i[1] for i in n) / len(n)
        l = (nx**2 + ny**2)**0.5
        nx, ny = nx / l, ny / l

        hx, hy = v[0] + nx * s, v[1] + ny * s
        sx, sy = v[0] + nx * 0.2, v[1] + ny * 0.2

        ax.plot([sx, hx], [sy, hy], lw=1.5, color='black')
        ax.plot(hx, hy, 'o', ms=5, mfc='white', mec='black')

# ---------- TEXT ----------
t = g + 1
val = poly_val(t)

omega_val = val["Omega'"]
theta_val = val["Theta'"]
pi_val = val["Pi'"]
sd_val = val["Sd'"]

def f(x):
    return f"{int(x)}" if abs(x - int(x)) < 1e-9 else f"{x:.2f}"

top = (
    f"Polynomial Equations:\n\n"
    f"Omega(G2,x) = {fmt(E1(t))}\n\n"
    f"Theta(G2,x) = {fmt(E2(t))}\n\n"
    f"Pi(G2,x) = {fmt(E3(t))}\n\n"
    f"Sd(G2,x) = {fmt(E4(t))}"
)

bottom = (
    f"Index Values:\n\n"
```

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```
        f"Omega' = {f(omega_val)}\n\n"
        f"Theta' = {f(theta_val)}\n\n"
        f"Pi' = {f(pi_val)}\n\n"
        f"Sd' = {f(sd_val)}"
    )

    fig.text(0.65, 0.85, top, fontsize=9, bbox=dict(boxstyle='round', fc='white'))
    fig.text(0.65, 0.25, bottom, fontsize=10, bbox=dict(boxstyle='round', fc='white'))

    ax.set_title(f"Triangular Nanographene (gamma = {t})")
    plt.show()


g = int(input("Enter dimension gamma: "))
draw(g - 1)
```

9 Sample Output for Triangular nanographene with Pendant Edges

The above Python implementation is executed for the dimension $\gamma = 5$ to generate the corresponding graph structure and compute the associated counting polynomials and topological indices. The results are obtained within a computational time of seven seconds, demonstrating the efficiency of the proposed approach. The sample output obtained from the program is presented below.

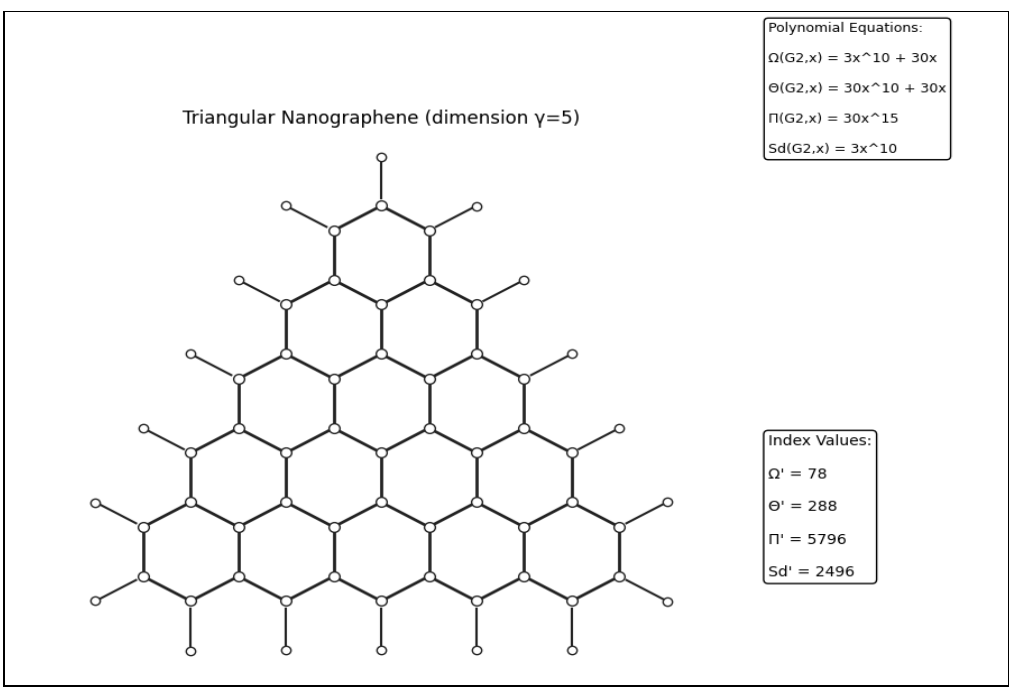

Figure 11: Python-based visualization and verification of the triangular nanographene structure, counting

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polynomials, and corresponding indices for dimension $\gamma = 5$.

10 Conclusion

Conclusion. The development of advanced materials for energy storage, optoelectronic devices (such as field-effect transistors, LEDs, and solar cells), and nanoelectronic applications places graphene and nanographene structures with pendant edges at the forefront of current research. In this study, nanographene and triangular nanographene structures with pendant edges were systematically constructed and analyzed using edge-cut techniques, and the corresponding counting polynomials, namely the Omega, Theta, Pi, and Sadhana polynomials, along with their associated topological indices, were derived. These polynomial-based indices provide meaningful insights into key physicochemical properties such as thermal stability, electronic behavior, charge mobility, and chemical reactivity. Based on the derived theoretical results, Python code was implemented to efficiently generate the corresponding structures, counting polynomials, and topological indices in a short time, thereby improving computational efficiency and reproducibility. This study contributes to Sustainable Development Goal 9 (Industry, Innovation and Infrastructure) by enabling efficient computational design and analysis of nanographene-based materials, and also supports SDG 12 (Responsible Consumption and Production) by reducing reliance on costly and resource-intensive experimental methods through predictive mathematical modeling. Future work may extend this approach to larger and more complex graphene-based systems, which may exhibit enhanced electronic and optoelectronic properties and broaden their potential applications in advanced technologies.

Disclosure of Interest

No potential conflict of interest was reported by the authors.

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