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Research Article

Omega, Sadhana, and *PI* Polynomials of Porous Graphene

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Abstract: Recently, graphene has become a significant and interesting substance. Many researchers have studied graphene-related materials in extensive detail both theoretically and practically, drawn by its exceptional features. The collection of graphene-bound materials that contain in-plane nanopores is called porous graphene, which exhibits structural and electrochemical properties distinct from pure ones. Porous graphene large surface area and excellent conductivity render it optimal for battery and supercapacitor energy retention biosensors, DNA sequencing, hydrogen storage and gas separation. Where Omega, Sadhana, and *PI* polynomials optimize charge distribution and energy density for better performance in devices like electric vehicles and smartphones. The present work concentrates on obtaining the polynomials Omega, Sadhana, and *PI* that are based on quasi-orthogonal cuts which are related to certain properties and express graph topological invariants.

Keywords: topological index, Omega polynomial, sadhana polynomial, Padmakar-Ivan polynomial, porous graphene, quasi-orthogonal cuts

1. Introduction

A graph can be depicted as a matrix, an array of numbers, a solitary value (frequently referred to as topological index), or an algebraic expression. These polynomials are influenced by chemical graph characteristics, including matching collections, independent subsets, chromatic indices, and equidistant connections. In chemical graph theory, we frequently represent a molecular structure using a graph, where the atoms are symbolized by vertices and the bonds by edges linking them [1–3]. In chemical graph theory, we frequently represent a molecular structure using a graph, where the atoms are symbolized by vertices and the bonds by edges linking them [1–3].

First proposed the concept of counting polynomials in 1936 by Polya [4]. For a very long period, chemists paid little attention to this idea. Nevertheless, comprehensive computational investigations into the analysis of the spectrum of the characteristic polynomial of graphs were conducted to identify the molecular orbitals of unsaturated hydrocarbons.

A graph F is an ordered pair $F = (N(F),\ B(F))$, where $N(F)$ is the the vertex set and $B(F)$ is the edges set, free from loops and multiple edges. The least number of edges in the path between two vertices u and v, given by the symbol $d(u,\ v)$, is the distance between them. A distance-counting polynomial was formulated by Hosoya as [5]:

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$$P(F,\ x) = \sum_{r} m(F,\ r)x^{r}$$

By $m(F,\ r)$, we mean the number of strips of length r of each other with $m(F,\ 0) = |N(F)|$ and $m(F,\ 1) = |B(F)|$. Two edges $h = v_1v_2$ and $g = u_1u_2$ of F are called codistant, "$h\ Co\ g$", if and only if $d(v_1,\ u_1) = d(v_2,\ u_2)$ and $d(v_1,\ u_2) = d(u_1,\ v_2) = d(v_1,\ u_1) + 1$. The relation "co" is evidently reflexive and symmetric, but transitivity is not a necessary property. If two edges h and g are the opposing edges of an inner face of a planar graph F, they are in relation opposite, denoted by "$h\ op\ g$". Keep in mind that the relation op is only defined in faces. The relation operation divides the set of $B(F)$ into opposing edge strip operations. Consider $S(h) = \{g \in B(F) : g\ Co\ h\}$ the collection of all the edge's co-distances of $h \in B(F)$. The relationship is referred to as a quasi-orthogonal cut if the relation "Co" is transitive on $S(h)$, then $S(h)$ is an orthogonal cut of the graph F denoted by "OC". If it is not transitive, the relation will be quasi orthogonal cut (QOC). The graph F is referred to as a co-graph if and only if the edge set $B(F)$ is a collection of non-overlapping orthogonal divisions. In general, the relationship between "ops" and "qoc" defies the transitivity theory (quasi-orthogonal cuts). The definitions of the polynomials Omega, Sadhana, and PI are based on quasi-orthogonal cuts. For non negative integer r, let $\phi(F,\ r)$ stand for the number of $QOCs$ of length r. Diudea introduced the Omega polynomial [6] denoted by $\omega(F,\ x)$ and defined as

$$\omega(F,\ x) = \sum_{r} \phi(F,\ r)x^{r}$$

The first derivative of Omega polynomial at $x = 1$ equals the number of edges in the graph

$$\omega'(F,\ x)|_{x=1} = \sum_{r} \phi(F,\ r)r = |B(F)|$$

Sadhana polynomial was inroduced by Ashrafi et al. [7] represented by $Sd(F,\ x)$ is related to "ops" of graph F and counts the nonopposite edges in F and defined as

$$Sd(F,\ x) = \sum_{r} \phi(F,\ r)x^{|B(F)|-r}$$

The Padmakar-Ivan polynomial $PI(F,\ x)$ was proposed by Khadikar et al. [8], which count the opposite edge strips in graph F and is defined as

$$PI(F,\ x) = \sum_{r} \phi(F,\ r)r\ x^{|B(F)|-r}$$

Chemical graph theory scholars have been interested in counting polynomials which introduced into this theory by either as approximations to solutions of the Schrödinger equation, or by encoding data in a mathematical structure andattempting to discern consistency in the roots of these expressions. Exponents indicate the size of a property, while coefficients indicate the number of times the property occurs and some recent work is found in [9]. The Omega polynomial, Sadhana polynomial, and PI polynomial of graphene the counting polynomials that we are looking for in this study. These three polynomials are dependent on the separation between chemical graph edges.

2. Results and discussion

Porous Graphene and counting polynomials. Figure 1 depicts the structure of Porous graphene $P[t,\ q]$. An edge made up of two carbon atoms connects six hexagons. Furthermore, the six hexagons are linearly connected by carbon-carbon atoms in both the row and the column [10, 11].

In general, if t and q, are the number of rows and columns respectively. It can be seen that $|N(P[t,\ q])| = 24tq + 12t$ and $|B(P[t,\ q])| = 30tq - q + 13t$. Moreover, there are $2q + 10t + 12tq$ vertices of degree 2 and $3t - 2q + 12tq$ of degree 3.

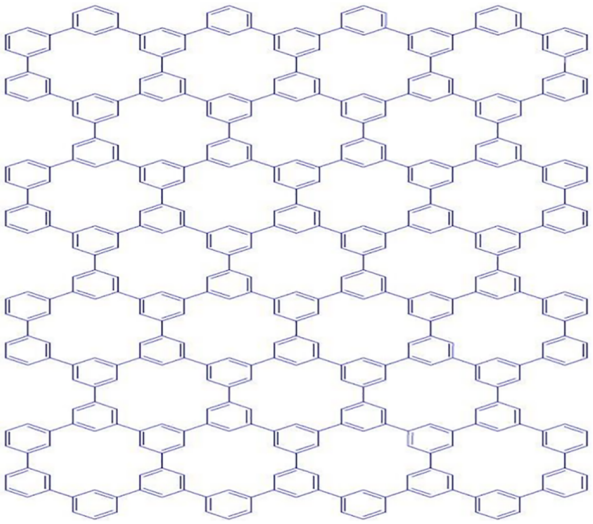

Figure 1. Porous graphene structure $P[4,\ 4]$

Theorem 1 The Omega polynomial of Porous Graphene Structure $P[t,\ q]$, if $t \geq q$ is as follows:
$\omega(P[t,\ q],\ x) = 12tqx^2 + 6tx^2 + x^q(tx + t - 1) + 2(t - q + 1)x^{2q} + 4\sum_{j=1}^{q-1} x^{2j}$. Similarly if $t < q$.

Proof. To calculate the omega polynomial of $P[t,\ q]$, we must determine the quasi-orthogonal cuts "qoc" and count the number of edges used in the "$qocs$". According to Figures 2 and 3, there are twelve different forms of "qoc" in a single unit cell of $P[t,\ q]$. So $\omega(P[1,\ 1],\ x) = 21x^2$.

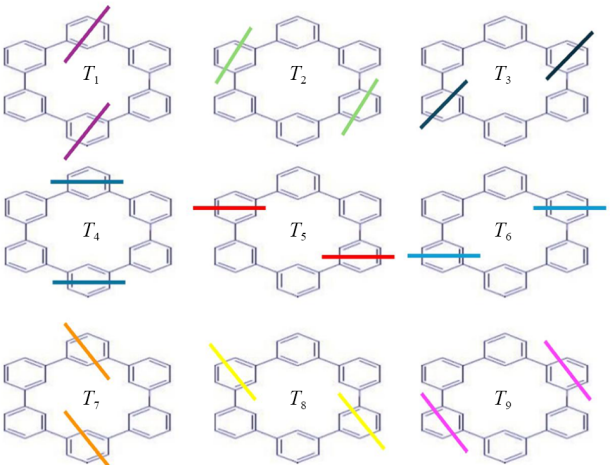

Figure 2. $T_i,\ 1 \leq i \leq 9$

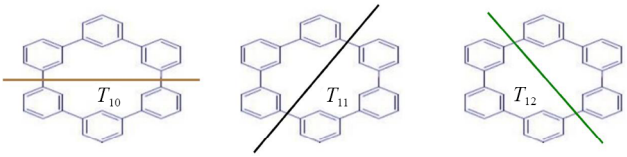

Figure 3. $T_i,\ 10 \leq i \leq 12$

These quasi orthogonal cuts can be applied to the entire graph as we show in Figures 4. Table 1 lists the overall number of these cuts as well as the total number of edges employed in these cuts.

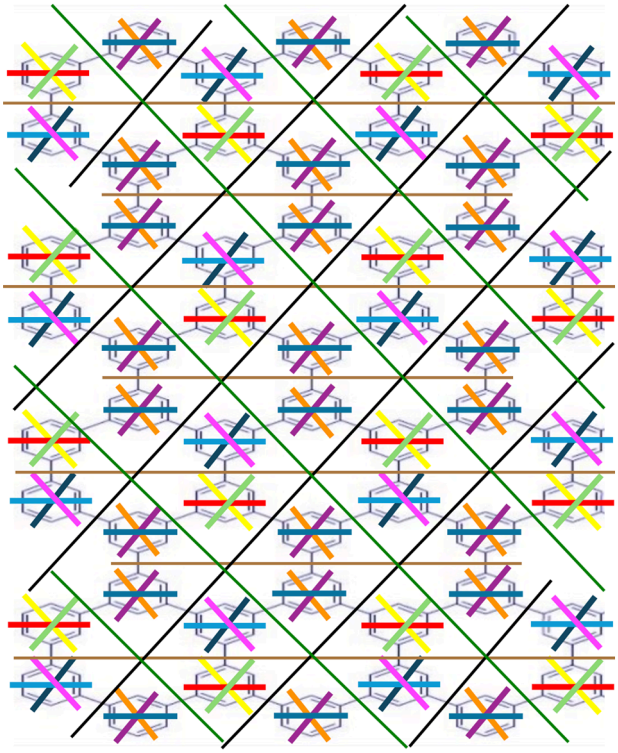

Figure 4. $T_i,\ 1 \leq i \leq 12$ of $P[4,\ 3]$

Table 1. Co-distant edges in $P[t,\ q], t \geq q$

Type of qocs	Number of codistant edges	Cardinality of strips of length r (qocs)
$T_i,\ i \in \{1,\ 4,\ 7\}$	2	$2tq$
$T_i,\ i \in \{2,\ 3,\ 5,\ 6,\ 8,\ 9\}$	2	$t(q+1)$
T_{10}	$q+1,\ q$	$t,\ t-1$
$T_i,\ i \in \{11,\ 12\}$	$2q,\ 2j, 1 \leq j \leq q-1$	$t-q+1,\ 2$

$$\omega(P[t,\ q],\ x) = 6t(q+1)x^2 + 3(2tq)x^2 + tx^{q+1} + (t-1)x^q + 2(t-q+1)x^{2q} + 4\sum_{j=1}^{q-1} x^{2j}$$

$$= 12tqx^2 + 6tx^2 + x^q(tx+t-1) + 2(t-q+1)x^{2q} + 4\sum_{j=1}^{q-1} x^{2j}$$

From theorem above, we get

$$\omega'(P[t,\ q],\ x)|_{x=1} = 24tq + 12t + t(q+1) + q(t-1) + 4q(t-q+1) + 8\sum_{j=1}^{q-1} j$$

$$= 24tq + 12t + tq + t + tq - q + 4tq - 4q^2 + 4q + 4q(q-1)$$

$$= 30tq + 13t - q = |B(P[t,\ q))|.$$

□

According to Figure 4, we compute the Omega polynomial of $P[4,\ 3]$ and we get

$$\omega(P[4,\ 3]) = 168x^2 + 4x^2 + 2x^4 + 2x^4 + 2x^6 + 2x^6 + 4x^4 + 3x^3$$

$$= 172x^2 + 3x^3 + 8x^4 + 4x^6$$

which matches the omega polynomial that we obtain in Theorem 1.1.

Theorem 2 The Sadhana polynomial of Porous Graphene Structure $P[t,\ q]$, if $t \geq q$ is given by:

$$Sd(P[t,\ q],\ x) = x^{30tq+13t-q}\Bigg(12tqx^{-2} + 6tx^{-2} + tx^{-(q+1)} + (t-1)x^{-q}$$

$$+ 2(t-q+1)x^{-2q} + 4\sum_{j=1}^{q-1} x^{-2j}\Bigg)$$

Proof. From the definition of Sadhana polynomial

$$Sd(F,\ x) = \sum_r \phi(F,\ r)x^{|B(F)|-r},\ |B(P[t,\ q])| = 30tq - q + 13t.$$

By replacing the number of quasi-orthogonal cuts and the value of codistant edges from Table 1, we get

$$Sd(P[t,\ q],\ x) = x^{30tq+13t-q}\Bigg(12tqx^{-2} + 6tx^{-2} + tx^{-(q+1)} + (t-1)x^{-q}$$

$$+ 2(t-q+1)x^{-2q} + 4\sum_{j=1}^{q-1} x^{-2j}\Bigg)$$

□

Theorem 3 The Padmakar-Ivan polynomial of Porous Graphene Structure $P[t,\ q]$, if $t \geq q$ is as follows:

$$PI(P[t,\ q],\ x) = x^{30tq+13t-q}\Bigg(24tqx^{-2} + 12tx^{-2} + t(q+1)x^{-(q+1)} + q(t-1)x^{-q}$$

$$+ 4q(t-q+1)x^{-2q} + 8\sum_{j=1}^{q-1} jx^{-2j}\Bigg).$$

Proof. Use Table 1 and substitute $|B(P[t,\ q])|$ by $30tq - q + 13t$ in definition of the Padmakar-Ivan to get

$$PI(P[t,\ q],\ x) = x^{30tq+13t-q}\Bigg(24tqx^{-2} + 12tx^{-2} + t(q+1)x^{-(q+1)} + (t-1)qx^{-q}$$

$$+ 4q(t-q+1)x^{-2q} + 8\sum_{j=1}^{q-1} jx^{-2j}\Bigg).$$

To compute the PI index of Porous Graphene, we evaluate the derivative of PI polynomial at $x = 1$,

$$PI'(P[t,\ q],\ x)|_{x=1} = 12(2tq+t)(30tq+13t-q-2) + t(q+1)(30tq+13t-2q-1)$$

$$+ q(t-1)(30tq+13t-2q) + 4q(t-q+1)(30tq+13t-3q) + 8\sum_{j=1}^{q-1} j(30tq+13t-q-2j)$$

□

3. Conclusion

Counting polynomials are an effective approach for representing the topological indices of chemical graphs, commonly utilized in structure-activity relationships and as measures of various physicochemical properties of compounds.

Conflict of interest

The authors declare no competing financial interest.

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