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Computation of Neighborhood *M*-Polynomial of Octa-Graphene 2D Nanosheet

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Abstract

Carbon-based two-dimensional nanosheets, including the recently discovered Octa-graphene, have emerged as promising materials with diverse applications. To fully understand their properties and potential, it is crucial to explore their topological indices. In this work, we delve into the derivation of the neighborhood *M*-polynomial for Octa-graphene. This polynomial enables the calculation of neighborhood degree-based topological indices, which are valuable tools for predicting various physical and chemical properties of the material. By employing these indices, we can gain deeper insights into the structure-property relationships of Octa-graphene and other similar nanosheets.

Keywords: 2D carbon nanosheets, Octa-graphene, Molecular structure, Neighborhood *M* -polynomial.

Introduction

Chemical graph theory is a field that blends mathematics and chemistry. It involves representing molecules as graphs, which are mathematical structures composed of nodes (atoms) and edges (bonds) [1]. By analyzing these molecular graphs, researchers can calculate numerical values called topological indices. These indices provide insights into the structural properties of molecules, which in turn can be correlated with their physical, chemical, and biological properties. One of the earliest applications of topological indices was in 1947, when Wiener [2] used them to predict the physical properties of molecules. Since then, topological indices have become invaluable tools in various areas of chemistry, including drug discovery and materials science [3, 4].

Topological indices can be categorized based on the specific structural features they highlight. Distance-based indices focus on interatomic distances, while degree-based indices consider the number of bonds connected to each atom. Connectivity indices capture the branching patterns of the molecular graph, and information-theoretic indices quantify the information content encoded within the structure [5]. To efficiently calculate these indices, algebraic polynomials, such as M-polynomials, have been employed [6]. These polynomials streamline the derivation of topological indices, particularly degree-based indices. Building upon this, Mondal et al. introduced the neighborhood *M*-polynomial (*NM*-polynomial), a powerful tool for calculating neighborhood degree-based indices [7].

Researchers have employed the neighborhood M-polynomial to investigate a wide range of molecular structures, including crystallographic structures [8], titanium compounds [9], polycyclic aromatic hydrocarbons [10], Polymers [11], fractals [12], dendrimers [13], metal-organic networks [14], silicon carbide networks [15], graphene networks [16], cycloparaphenylenes [17], supercoronene [18], porphyrazine [19], nanotube [20] and nanostructures [21]. By applying this polynomial, researchers have been able to compute and analyze various topological indices, such as the neighborhood second-modified Zagreb index, the neighborhood harmonic index, and degree-sum-based indices. These indices have shown promise in predicting properties like molar refractivity, polarizability, molar volume, and other relevant characteristics of molecules [22,23].

Carbon-based nanomaterials, especially two-dimensional (2D) nanosheets, are reshaping the landscape of nanotechnology. Graphene, a prime example, is a single layer of carbon atoms arranged in a hexagonal lattice [24]. Its exceptional strength, flexibility, and electrical conductivity have captured the attention of researchers worldwide [25, 26]. Another fascinating 2D carbon-based nanomaterial is octa-graphene, composed of octagons and squares. This unique structure, formed from butadienes and linear carbon chains, can be rolled up into nanotubes, opening up new possibilities for its applications [27]. The degree-based topological properties of Octa-graphene were explored through *M*-polynomial in [28]. Given the significant importance of Octa-graphene structures, further theoretical structural analysis is required. Therefore, in this article, we delve into the study of Octa-graphene structures using neighborhood degree-based polynomial techniques. The rest of the manuscript is structured as follows. Section 2 presents the necessary preliminaries and methodology for obtaining the main results. Section 3 focuses on the computation of the neighborhood *M*-polynomial of octa-graphene. Finally, Section 4 concludes the work.

Preliminaries:

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$. Also let $|V(G)|$ and $|E(G)|$ be the order and size of G. The degree of vertex $u \in V(G)$ is denoted by $d(u)$ and is the number of vertices that are adjacent to u and $nd(u)$ denote the degree sum of all vertices of G that are adjacent to u known as neighborhood degree sum of u in G. The neighborhood *M*-polynomial of the graph is defined as,

$$NM(G; x, y) = \sum_{i \le j} m^*_{ij}(G) x^i y^j \qquad \text{where,}$$

$$m^*_{ij}(G), i, j \ge 1, \text{is the number of edges } uv \text{ of } G \text{ such that } \{(nd(u), nd(v)) = \{i, j\}\}$$

Table 1 lists specific neighborhood degree-based topological indices of graph G, which are derived using the *NM*-polynomial through calculus.

Topological Index	**Formula** $g(\chi(u),\chi(v))$	**Derivation from** $f(x,y)$ $f(x,y) = NM(G;x,y)$
Third version Zagreb index: $NM_1(G)$	$\sum_{uv\in E(G)} (\chi(u)+\chi(v))$	$(D_x + D_y)(f(x,y))_{x=y=1}$
Neighborhood second Zagreb index: $NM_2(G)$	$\sum_{uv\in E(G)} \chi(u)\chi(v)$	$(D_x D_y)(f(x,y))_{x=y=1}$
Neighborhood Second modified Zagreb index: $NmM_2(G)$	$\sum_{uv\in E(G)} \frac{1}{\chi(u)\chi(v)}$	$(S_x S_y)(f(x,y))_{x=y=1}$
Third NDe index: $ND_3(G)$	$\sum_{uv\in E(G)} \chi(u)\chi(v)(\chi(u)+\chi(v))$	$D_x D_y(D_x + D_y)(f(x,y))_{x=y=1}$
Neighborhood Forgotten topological index: $NF(G)$	$\sum_{uv\in E(G)} (\chi^2(u)+\chi^2(v))$	$({D_x}^2 + {D_y}^2)(f(x,y))_{x=y=1}$
Neighborhood Randić index: $NR_k(G)$	$\sum_{uv\in E(G)} (\chi(u)\chi(v))^k$	$({D_x}^k {D_y}^k)(f(x,y))_{x=y=1}$
Neighborhood Inverse Randić index: $NRR_k(G)$	$\sum_{uv\in E(G)} \frac{1}{(\chi(u)\chi(v))^k}$	$({S_x}^k {S_y}^k)(f(x,y))_{x=y=1}$
Fifth NDe index: $ND_5(G)$	$\sum_{uv\in E(G)} \frac{\chi^2(u)+\chi^2(v)}{\chi(u)\chi(v)}$	$(D_x S_y + S_x D_y)(f(x,y))_{x=y=1}$
Neighborhood Harmonic Index: $NH(G)$	$\sum_{uv\in E(G)} \frac{2}{\chi(u)+\chi(v)}$	$(2S_x J)(f(x,y))_{x=1}$
Neighborhood Inverse sum Index: $NI(G)$	$\sum_{uv\in E(G)} \frac{\chi(u)\chi(v)}{(\chi(u)+\chi(v))}$	$(S_x J D_x D_y)(f(x,y))_{x=1}$
Sanskruti Index: $S(G)$	$\sum_{uv\in E(G)} \left\{\frac{\chi(u)\chi(v)}{\chi(u)+\chi(v)-2}\right\}^3$	$({S_x}^3 Q_{-2} J {D_x}^3 {D_y}^3)(f(x,y))_{x=1}$
Fifth hyper $M_1(G)$ Zagreb index $NHM_1G_5(G)$	$\sum_{uv\in E(G)} (\chi(u)+\chi(v))^2$	$({D_x}^2 + {D_y}^2 + 2D_x D_y)(f(x,y))_{x=y=1}$
Fifth hyper $M_2(G)$ Zagreb index $NHM_2G_5(G)$	$\sum_{uv\in E(G)} (\chi(u)\chi(v))^2$	$D_x D_y(D_x D_y)(f(x,y))_{x=y=1}$

Fifth arithmetic-geometric index $NAG_5(G)$	$\sum_{uv\in E(G)} \frac{(\chi(u)+\chi(v))}{2\sqrt{\chi(u)\chi(v)}}$	$\frac{1}{2}S_x^{\frac{1}{2}}S_y^{\frac{1}{2}}(D_x+D_y)(f(x,y))_{x=y=1}$
Fifth geometric- arithmetic index $NGA_5(G)$	$\sum_{uv\in E(G)} \frac{2\sqrt{\chi(u)\chi(v)}}{(\chi(u)+\chi(v))}$	$2S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}}(f(x,y))_{x=y=1}$
Where $D_x = x\left(\frac{\partial(f(x,y))}{\partial x}\right), D_y = y\left(\frac{\partial(f(x,y))}{\partial y}\right), S_x = \int_0^x \frac{f(t,y)}{t}dt, S_y = \int_0^y \frac{f(x,t)}{t}dt, J(f(x,y)) = f(x,x),\ Q_k(f(x,y)) = x^k f(x,y)$ *For neighborhood degree based topological indices:* $\chi(u) = nd(u),\ \chi(v) = nd(v),\ f(x,y) = NM(G;x,y)$		

Table 1: Description of neighborhood degree-based topological indices and their derivation from NM-polynomial.

To compute the *NM*-polynomial of Octa-graphene, we first constructed specific molecular graphs of Octa-graphene. We represent the graph of an Octa-graphene nanosheet as $OG_{m\times n}$, where *m* and *n* denote the number of octagons in each row and column, respectively. Figure 1 illustrates small graphs of Octa-graphene $OG_{1\times 1}$, $OG_{2\times 2}$ and $OG_{4\times 4}$, as well as the growth pattern of this nanosheet.

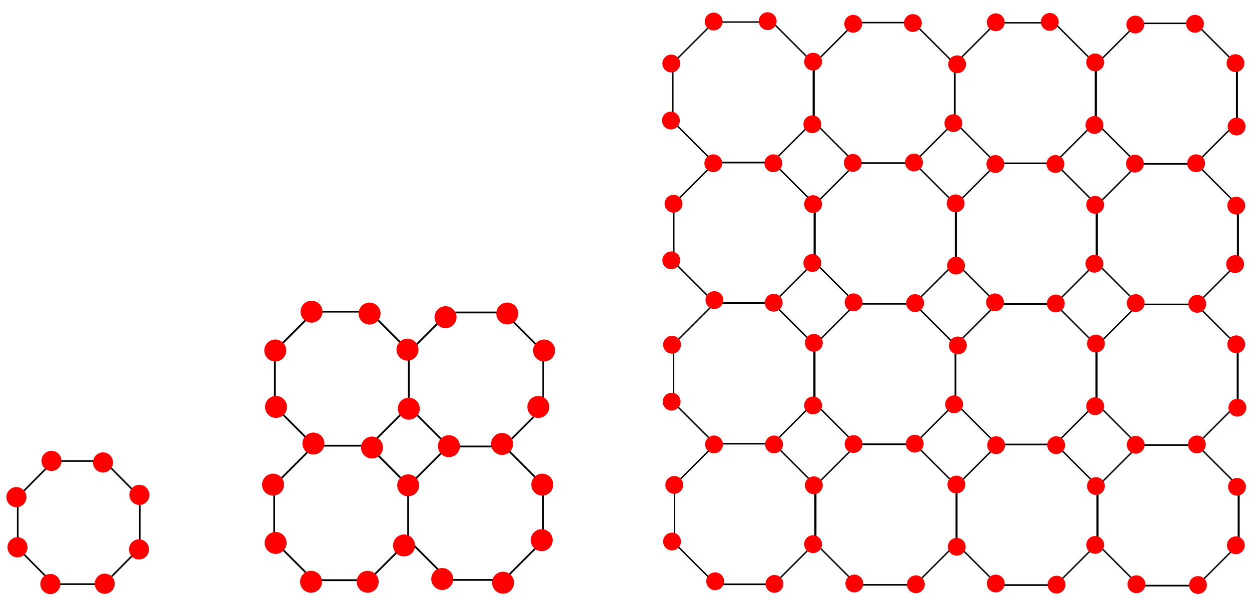


Figure 1: Graphs of $OG_{1\times 1}$, $OG_{2\times 2}$ and $OG_{4\times 4}$

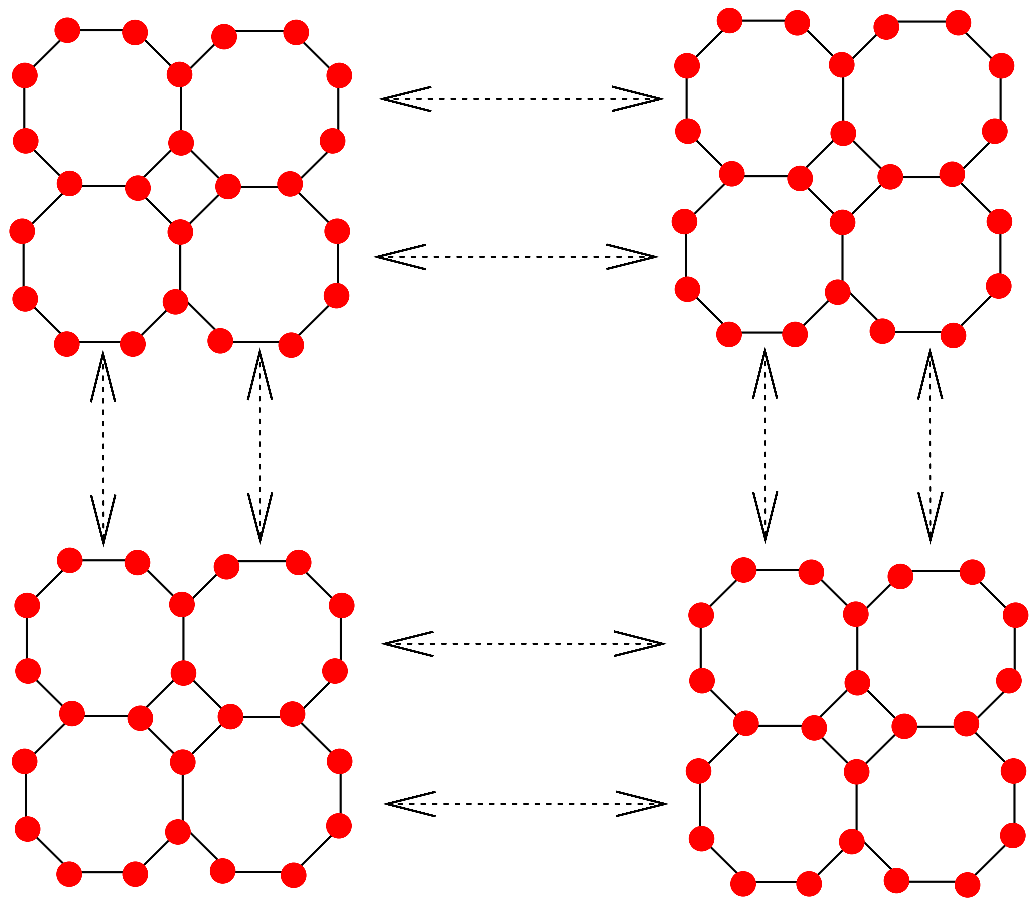


Figure 2: Graph of Octa graphene $OG_{m\times n}$

Main Results

This section presents various neighborhood degree-based topological indices of Octa-graphene, obtained using the *NM*-polynomial. The primary results discussed in this section are as follows:

Theorem 1: Let $OG_{m\times n}$ be the graph of Octa-graphene nanosheet, then *NM*-polynomial for $OG_{m\times n}$ is given as for $m > 1, n > 1$

$$NM(OG_{m\times n}; x, y) = 4x^4y^4 + 8x^4y^5 + 2(m+n-2)x^5y^5 + 4(m+n-2)x^5y^7$$
$$+2(m+n-2)\,x^7y^9 + 2(3m^2-7n+4)\,x^9y^9.$$

Proof: By the growth pattern of Octa-graphene graph as shown in Figure 1 and Figure 2, we observe that the graph of $OG_{m\times n}$ has $4mn+2m+2n$ vertices and $6mn+m+n$ edges, where *m* and *n* are the number of rows and columns in Figure 2. The neighborhood degree of vertices of $OG_{m\times n}$ are 4, 5, 7 and 9 therefore six partitions for the edge set based on the neighborhood degree are $(4,4),(4,5)$,

$(5,5),(5,7),(7,9),(9,9)$.Let $E^*_{ij}=\{uv\in E(OG_{m\times n})|nd(u)=i,nd(v)=j\}$

on the basic of neighborhood degree of vertices, the edge set of $OG_{m\times n}$ can be divided into six classes as follows

$$E_{44}=\{uv\in E(OG_{m\times n})|nd(u)=4,nd(v)=4\},$$

$$E_{45}=\{uv\in E(OG_{m\times n})|nd(u)=4,nd(v)=5\},$$

$$E_{55}=\{uv\in E(OG_{m\times n})|nd(u)=5,nd(v)=5\},$$

$$E_{57}=\{uv\in E(OG_{m\times n})|nd(u)=5,nd(v)=7\},$$

$$E_{79}=\{uv\in E(OG_{m\times n})|nd(u)=7,nd(v)=9\},$$

$$E_{99}=\{uv\in E(OG_{m\times n})|nd(u)=9,nd(v)=9\},$$

and

$|E_{44}|=4, |E_{45}|=8, |E_{55}|=2(m+n-2), |E_{57}|=4(m+n-2),$

$|E_{79}|=2(m+n-2), |E_{99}|=2(3m^2-7n+4).$

Using definition of *NM*-polynomial

$$NM(G;x,y)=\sum_{i\le j} m^*_{ij}\,(G)x^iy^j$$

$$NM(OG_{m\times n};x,y)=\sum_{4\le 4} m^*_{44}\,x^4y^4+\sum_{4\le 5} m^*_{45}\,x^4y^5+\sum_{5\le 5} m^*_{55}\,x^5y^5+\sum_{5\le 7} m^*_{57}\,x^5y^7$$
$$+\sum_{7\le 9} m^*_{79}\,x^7y^9\ +\sum_{9\le 9} m^*_{99}\,x^9y^9.$$

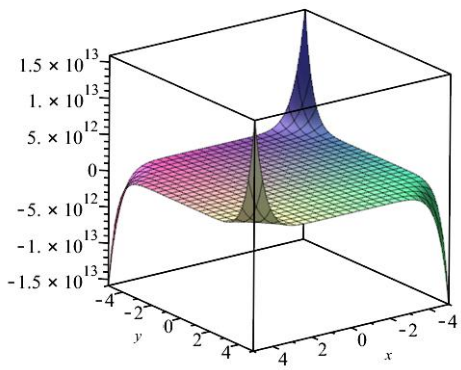
$NM(OG_{m\times n};x,y)=|E_{44}|x^4y^4+\ |E_{45}|x^4y^5+\ |E_{55}|x^5y^5\ +\ |E_{57}|x^5y^7+\ |E_{79}|x^7y^9$

$$+ |E_{99}| x^9 y^9.$$

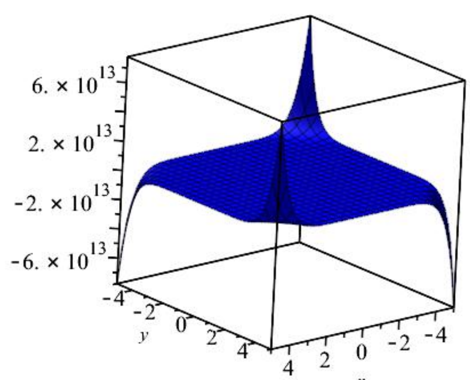
$$NM(OG_{m\times n}; x, y) = 4x^4y^4 + 8x^4y^5 + 2(m+n-2)x^5y^5 + 4(m+n-2)x^5y^7$$
$$+2(m+n-2)\, x^7y^9 + 2(3m^2 - 7n + 4)\, x^9y^9.$$

Hence, the result is obtained.

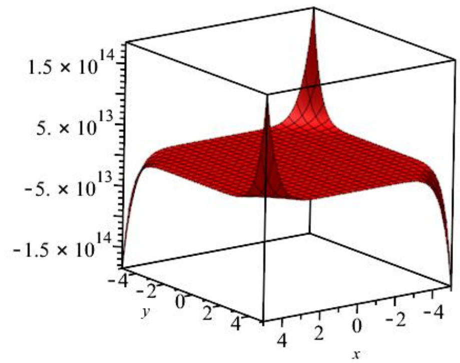
The surface representations of *NM*-polynomials of $OG_{2\times 2}, OG_{3\times 3}$ and $OG_{4\times 4}$ are shown in Figure 3.



$$NM(OG_{2\times 2}; x, y) = 4x^4y^4 + 8x^4y^5 + 4x^5y^5 + 8x^5y^7 + 4x^7y^9 + 4\, x^9y^9.$$



$$NM(OG_{3\times 3}; x, y) = 4x^4y^4 + 8x^4y^5 + 8x^5y^5 + 16x^5y^7 + 8x^7y^9 + 20\, x^9y^9.$$



$$NM(OG_{4\times 4};x,y) = 4x^4y^4 + 8x^4y^5 + 12x^5y^5 + 24x^5y^7 + 12x^7y^9 + 48x^9y^9.$$

Figure 3: The NM-polynomial for $OG_{2\times 2}, OG_{3\times 3}$ and $OG_{4\times 4}$ respectively.

Now using this NM-polynomial, some neighborhood degree-based topological indices of $OG_{m\times n}$ are obtained in the following theorem.

Theorem 2: Let $OG_{m\times n}$ be the graph of Octa-graphene nanosheet, then for $m > 1, n > 1$

1. $NM_1(OG_{m\times n}) = 108m^2 + 100m - 152n + 48.$

2. $NM_2(OG_{m\times n}) = 486m^2 + 316m - 818n + 244.$

3. $NmM_2(OG_{m\times n}) = \frac{2}{27}m^2 + \frac{356}{1575}m + \frac{754}{14175}n + \frac{16823}{56700}$

4. $ND_3(OG_{m\times n}) = 8748m^2 + 4196m - 16216n + 5224.$

5. $NF(OG_{m\times n}) = 972m^2 + 656m - 1612n + 440.$

6. $NR_k(OG_{m\times n}) = (4)^{2k+1} + (20)^k\, 8 + (25)^k 2(m+n-2) + (35)^k 4(m+n-2) + (63)^k 2(m+n-2) + (81)^k 2(3m^2 - 7n + 4).$

7. $NRR_k(OG_{m\times n}) = \frac{4}{(4)^{2k}} + 8\frac{8}{(20)^k} + \frac{2(m+n-2)}{(25)^k} + \frac{4(m+n-2)}{(35)^k} + \frac{2(m+n-2)}{(63)^k} + \frac{2(3m^2-7n+4)}{(81)^k}.$

8. $ND_5(OG_{m\times n}) = 12m^2 + 16.58413m - 11.41587n + 7.23175$

9. $NH(OG_{m\times n}) = 0.66666m^2 + 1.31666m - 0.23888n + 1.03333$

10. $NI(OG_{m\times n}) = 27m^2 + \frac{589}{24}m - \frac{923}{24}n + \frac{457}{36}$

11. $S(OG_{m\times n}) = \frac{129140163}{2048}m^2 + \frac{4866593}{256}m - \frac{262394303}{2048}n + \frac{241826917177}{4741632}$

12. $NHM_1G_5(OG_{m\times n}) = 1944m^2 + 1288m - 3248n + 920$

13. $NHM_2G_5(OG_{m\times n}) = 39366m^2 + 14088m - 77766n + 28536$

14. $NAG_5(OG_{m\times n}) = 6m^2 + 2m - 12n + \frac{24m+24n-48}{\sqrt{35}} + \frac{256m+256n-512}{\sqrt{63}} + 8 + \frac{36}{\sqrt{20}}.$

15. $NGA_5(OG_{m\times n}) = 6m^2 + 2m - 12n + \frac{2\sqrt{35}(m+n-2)}{3} + \frac{\sqrt{72}(m+n-2)}{4} + 8 + \frac{16\sqrt{20}}{9}.$

Proof: Let $f(x,y) = NM(OG_{m\times n}; x,y) = 4x^4y^4 + 8x^4y^5 + 2(m+n-2)x^5y^5$

$+4(m+n-2)x^5y^7 + 2(m+n-2)\,x^7y^9 + 2(3m^2-7n+4)\,x^9y^9.$

then

$D_xf(x,y) = 16x^4y^4 + 32x^4y^5 + 10(m+n-2)x^5y^5 + 20(m+n-2)x^5y^7$

$+ 14(m+n-2)\,x^7y^9 + 18(3m^2-7n+4)\,x^9y^9.$

$D_yf(x,y) = 16x^4y^4 + 40x^4y^5 + 10(m+n-2)x^5y^5 + 28(m+n-2)x^5y^7$

$+ 18(m+n-2)\,x^7y^9 + 18(3m^2-7n+4)\,x^9y^9$

$(D_x + D_y)(f(x,y))$

$= 32x^4y^4 + 72x^4y^5 + 20(m+n-2)x^5y^5 + 48(m+n-2)x^5y^7$

$+ 32(m+n-2)\,x^7y^9 + 36(3m^2-7n+4)\,x^9y^9.$

$D_xD_yf(x,y) = 64x^4y^4 + 160x^4y^5 + 50(m+n-2)x^5y^5 + 140(m+n-2)x^5y^7$

$+ 126(m+n-2)\,x^7y^9 + 162(3m^2-7n+4)\,x^9y^9.$

$D_x^2f(x,y) = 64x^4y^4 + 128x^4y^5 + 50(m+n-2)x^5y^5 + 100(m+n-2)x^5y^7$

$+ 98(m+n-2)\,x^7y^9 + 162(3m^2-7n+4)\,x^9y^9.$

$$D_y^2 f(x,y) = 64x^4y^4 + 200x^4y^5 + 50(m+n-2)x^5y^5 + 196(m+n-2)x^5y^7$$
$$+ 162(m+n-2)\,x^7y^9 + 162(3m^2-7n+4)\,x^9y^9.$$

$$\left(D_x^2 + D_y^2\right)\left(f(x,y)\right) = 128x^4y^4 + 328x^4y^5 + 100(m+n-2)x^5y^5$$
$$+296(m+n-2)x^5y^7 + 260(m+n-2)\,x^7y^9 + 324(3m^2-7n+4)\,x^9y^9.$$

$$D_x^k D_y^k f(x,y) = (4)^k(4)^k 4x^4y^4 + (4)^k(5)^k\,8x^4y^5 + (5)^k(5)^k 2(m+n-2)x^5y^5$$
$$+ (5)^k(7)^k 4(m+n-2)x^5y^7 + (7)^k(9)^k 2(m+n-2)\,x^7y^9$$
$$+ (9)^k(9)^k 2(3m^2-7n+4)\,x^9y^9.$$

$$D_y\left(D_x + D_y\right)\left(f(x,y)\right) = 128x^4y^4 + 360x^4y^5 + 100(m+n-2)x^5y^5$$
$$+336(m+n-2)x^5y^7 + 288(m+n-2)\,x^7y^9 + 324(3m^2-7n+4)\,x^9y^9$$

$$D_xD_y\left(D_x + D_y\right)\left(f(x,y)\right) = 512x^4y^4 + 1440x^4y^5 + 500(m+n-2)x^5y^5 +$$
$$1680(m+n-2)x^5y^7 + 2016(m+n-2)\,x^7y^9 + 2916(3m^2-7n+4)\,x^9y^9.$$

$$S_y f(x,y) = 4x^4\frac{y^4}{4} + 8x^4\frac{y^5}{5} + 2(m+n-2)x^5\frac{y^5}{5} + 4(m+n-2)x^5\frac{y^7}{7}$$
$$+ 2(m+n-2)\,x^7\frac{y^9}{9} + 2(3m^2-7n+4)\,x^9\frac{y^9}{9}.$$

$$S_xS_y f(x,y) = 4\frac{x^4}{4}\frac{y^4}{4} + 8\frac{x^4}{4}\frac{y^5}{5} + 2(m+n-2)\frac{x^5}{5}\frac{y^5}{5} + 4(m+n-2)\frac{x^5}{5}\frac{y^7}{7}$$
$$+ 2(m+n-2)\,\frac{x^7}{7}\frac{y^9}{9} + 2(3m^2-7n+4)\,\frac{x^9}{9}\frac{y^9}{9}.$$

$$S_x^k S_y^k f(x,y) = 4\frac{x^4}{(4)^k}\frac{y^4}{(4)^k} + 8\frac{x^4}{(4)^k}\frac{y^5}{(5)^k} + 2(m+n-2)\frac{x^5}{(5)^k}\frac{y^5}{(5)^k}$$
$$+ 4(m+n-2)\frac{x^5}{(5)^k}\frac{y^7}{(7)^k} + 2(m+n-2)\,\frac{x^7}{(7)^k}\frac{y^9}{(9)^k}$$
$$+ 2(3m^2-7n+4)\,\frac{x^9}{(9)^k}\frac{y^9}{(9)^k}.$$

$$S_x f(x,y) = 4\frac{x^4}{4}y^4 + 8\frac{x^4}{4}y^5 + 2(m+n-2)\frac{x^5}{5}y^5 + 4(m+n-2)\frac{x^5}{5}y^7$$

$$+ 2(m+n-2)\ \frac{x^7}{7}y^9 + 2(3m^2-7n+4)\frac{x^9}{9}y^9.$$

$$D_y S_x f(x,y) = 16\frac{x^4}{4}y^4 + 40\frac{x^4}{4}y^5 + 10(m+n-2)\frac{x^5}{5}y^5 + 28(m+n-2)\frac{x^5}{5}y^7$$

$$+ 18(m+n-2)\ \frac{x^7}{7}y^9 + 18(3m^2-7n+4)\frac{x^9}{9}y^9.$$

$$D_x S_y f(x,y) = 16x^4\frac{y^4}{4} + 32x^4\frac{y^5}{5} + 10(m+n-2)x^5\frac{y^5}{5} + 20(m+n-2)x^5\frac{y^7}{7}$$

$$+ 14(m+n-2)\ x^7\frac{y^9}{9} + 18(3m^2-7n+4)\ x^9\frac{y^9}{9}.$$

$$\left(D_x S_y + D_y S_x\right) f(x,y)$$

$$= 8x^4y^4 + \frac{82}{5}x^4y^5 + 4(m+n-2)x^5y^5 + \frac{296}{35}(m+n-2)x^5y^7$$

$$+ \frac{260}{63}(m+n-2)\ x^7y^9 + 4(3m^2-7n+4)\ x^9y^9.$$

$$Jf(x,y) = 4x^8 + 8x^9 + 2(m+n-2)x^{10} + 4(m+n-2)x^{12} + 2(m+n-2)\ x^{16}$$

$$+ 2(3m^2-7n+4)\ x^{18}.$$

$$S_x\, Jf(x,y) = 4\frac{x^8}{8} + 8\frac{x^9}{9} + 2(m+n-2)\frac{x^{10}}{10} + 4(m+n-2)\frac{x^{12}}{12} + 2(m+n-2)\ \frac{x^{16}}{16}$$

$$+ 2(3m^2-7n+4)\frac{x^{18}}{18}.$$

$$JD_yD_x f(x,y) = 64x^8 + 160x^9 + 50(m+n-2)x^{10} + 140(m+n-2)x^{12}$$

$$+ 126(m+n-2)\ x^{16} + 162(3m^2-7n+4)\ x^{18}.$$

$$S_xJD_yD_x f(x,y) = \frac{64}{8}x^8 + \frac{160}{9}x^9 + \frac{50}{10}(m+n-2)x^{10}$$

$$+\frac{140}{12}(m+n-2)x^{12}+\frac{126}{16}(m+n-2)\,x^{16}+\frac{162}{18}(3m^2-7n+4)\,x^{18}.$$

$$D_x^3D_y^3f(x,y)=(4)^3(4)^3 64x^4y^4+(4)^3(5)^3\,160x^4y^5+(5)^3(5)^3 50(m+n-2)x^5y^5$$

$$+(5)^3(7)^3 140(m+n-2)x^5y^7+(7)^3(9)^3 126(m+n-2)\,x^7y^9$$

$$+(9)^3(9)^3 162(3m^2-7n+4)\,x^9y^9.$$

$$JD_x^3D_y^3f(x,y)=(4)^3(4)^3 64x^8+(4)^3(5)^3\,160x^9+(5)^3(5)^3 50(m+n-2)x^{10}$$

$$+(5)^3(7)^3 140(m+n-2)x^{12}+(7)^3(9)^3 126(m+n-2)\,x^{16}$$

$$+(9)^3(9)^3 162(3m^2-7n+4)\,x^{18}.$$

$Q_{-2}JD_x^3D_y^3f(x,y)$

$$=(4)^3(4)^3 64x^6+(4)^3(5)^3\,160x^7+(5)^3(5)^3 50(m+n-2)x^8$$

$$+(5)^3(7)^3 140(m+n-2)x^{10}+(7)^3(9)^3 126(m+n-2)\,x^{14}$$

$$+(9)^3(9)^3 162(3m^2-7n+4)\,x^{16}$$

$S_x^3Q_{-2}JD_x^3D_y^3f(x,y)$

$$=(4)^3(4)^3(64)\frac{x^6}{(6)^3}+(4)^3(5)^3(\,160)\frac{x^7}{(7)^3}+(5)^3(5)^3(50)(m+n-2)\frac{x^8}{(8)^3}$$

$$+(5)^3(7)^3(140)(m+n-2)\frac{x^{10}}{(10)^3}+(7)^3(9)^3(126)(m+n-2)\;\frac{x^{14}}{(14)^3}$$

$$+(9)^3(9)^3(162)(3m^2-7n+4)\;\frac{x^{16}}{(16)^3}$$

$\left(D_x^2+D_y^2+2D_xD_y\right)\left(f(x,y)\right)$

$$=256x^4y^4+\;648x^4y^5+200(m+n-2)x^5y^5\;+576(m+n-2)x^5y^7$$

$$+512(m+n-2)\,x^7y^9+648(3m^2-7n+4)\,x^9y^9.$$

$D_yD_xD_yf(x,y)$

$$=256x^4y^4+\;800x^4y^5+250(m+n-2)x^5y^5\;+980(m+n-2)x^5y^7$$

$$+1134(m+n-2)\,x^7y^9+1458(3m^2-7n+4)\,x^9y^9.$$

$D_x D_y (D_x D_y) f(x,y)$

$$= 1024x^4y^4 + \ 3200x^4y^5 + 1250(m+n-2)x^5y^5 + 4900(m+n-2)x^5y^7$$

$$+ 7938(m+n-2)\ x^7y^9 + 13122(3m^2-7n+4)\ x^9y^9.$$

$S_y^{\frac{1}{2}}(D_x + D_y)(f(x,y))$

$$= 32x^4\frac{y^4}{\sqrt{4}} + \ 72x^4\frac{y^5}{\sqrt{5}} + 20(m+n-2)x^5\frac{y^5}{\sqrt{5}} + 48(m+n-2)x^5\frac{y^7}{\sqrt{7}}$$

$$+ 32(m+n-2)\ x^7\frac{y^9}{\sqrt{9}} + 36(3m^2-7n+4)\ x^9\frac{y^9}{\sqrt{9}}.$$

$S_x^{\frac{1}{2}} S_y^{\frac{1}{2}}(D_x + D_y)(f(x,y))$

$$= 32\frac{x^4}{\sqrt{4}}\frac{y^4}{\sqrt{4}} + \ 72\frac{x^4}{\sqrt{4}}\frac{y^5}{\sqrt{5}} + 20(m+n-2)\frac{x^5}{\sqrt{5}}\frac{y^5}{\sqrt{5}} + 48(m+n-2)\frac{x^5}{\sqrt{5}}\frac{y^7}{\sqrt{7}}$$

$$+ 32(m+n-2)\ \frac{x^7}{\sqrt{7}}\frac{y^9}{\sqrt{9}} + 36(3m^2-7n+4)\ \frac{x^9}{\sqrt{9}}\frac{y^9}{\sqrt{9}}.$$

$\frac{1}{2} S_x^{\frac{1}{2}} S_y^{\frac{1}{2}}(D_x + D_y)(f(x,y))$

$$= 16\frac{x^4}{\sqrt{4}}\frac{y^4}{\sqrt{4}} + \ 36\frac{x^4}{\sqrt{4}}\frac{y^5}{\sqrt{5}} + 10(m+n-2)\frac{x^5}{\sqrt{5}}\frac{y^5}{\sqrt{5}} + 24(m+n-2)\frac{x^5}{\sqrt{5}}\frac{y^7}{\sqrt{7}}$$

$$+ 16(m+n-2)\ \frac{x^7}{\sqrt{7}}\frac{y^9}{\sqrt{9}} + 18(3m^2-7n+4)\ \frac{x^9}{\sqrt{9}}\frac{y^9}{\sqrt{9}}.$$

$$D_x^{\frac{1}{2}} D_y^{\frac{1}{2}} f(x,y) = 16x^4y^4 + (\sqrt{20})\ 8x^4y^5 + 10(m+n-2)x^5y^5 \ + (\sqrt{35})4(m+n-2)x^5y^7$$

$$+ (\sqrt{72})2(m+n-2)\ x^7y^9 + 18(3m^2-7n+4)\ x^9y^9.$$

$$JD_x^{\frac{1}{2}} D_y^{\frac{1}{2}} f(x,y) = 16x^8 + (\sqrt{20})\ 8x^9 + 10(m+n-2)x^{10} \ + (\sqrt{35})4(m+n-2)x^{12}$$

$$+ (\sqrt{72})2(m+n-2)\ x^{16} + 18(3m^2-7n+4)\ x^{18}.$$

$$S_xJD_x^{\frac{1}{2}}D_y^{\frac{1}{2}}f(x,y) = 2x^8 + \frac{8}{9}(\sqrt{20})x^9 + (m+n-2)x^{10}$$

$$+\frac{(\sqrt{35})}{3}(m+n-2)x^{12} + \frac{(\sqrt{72})}{8}(m+n-2)\,x^{16} + (3m^2-7n+4)\,x^{18}$$

Now, using Table 1 we have

1. $NM_1(OG_{m\times n}) = \left(D_x + D_y\right)f(x,y)\big|_{x=y=1} = 108m^2 + 100m - 152n + 48.$

2. $NM_2(OG_{m\times n}) = D_xD_yf(x,y)\big|_{x=y=1} = 486m^2 + 316m - 818n + 244.$

3. $NmM_2(OG_{m\times n}) = S_xS_yf(x,y)\big|_{x=y=1} = \frac{2}{27}m^2 + \frac{356}{1575}m + \frac{754}{14175}n + \frac{16823}{56700}$

4. $ND_3(OG_{m\times n}) = D_xD_y(D_x + D_y)f(x,y)\big|_{x=y=1} = 8748m^2 + 4196m - 16216n + 5224.$

5. $NF(OG_{m\times n}) = (D_x^2 + D_y^2)(f(x,y))\big|_{x=y=1} = 972m^2 + 656m - 1612n + 440.$

6. $NR_k(OG_{m\times n}) = {D_x}^k{D_y}^kf(x,y)\big|_{x=y=1}$
$= (4)^{2k+1} + (20)^k\,8 + (25)^k2(m+n-2) + (35)^k4(m+n-2)$
$+ (63)^k2(m+n-2) + (81)^k2(3m^2-7n+4).$

7. $NRR_k(OG_{m\times n}) = {S_x}^k{S_y}^kf(x,y)\big|_{x=y=1}$

$$= \frac{4}{(4)^{2k}} + 8\frac{8}{(20)^k} + \frac{2(m+n-2)}{(25)^k} + \frac{4(m+n-2)}{(35)^k} + \frac{2(m+n-2)}{(63)^k}$$

$$+ \frac{2(3m^2-7n+4)}{(81)^k}.$$

8. $ND_5(OG_{m\times n}) = (D_xS_y + D_yS_x)f(x,y)\big|_{x=y=1}$

$$= 12m^2 + 16.58413m - 11.41587n + 7.23175$$

9. $NH(OG_{m\times n}) = 2S_xJ\,f(x,y)|_{x=y=1} = 0.66666m^2 + 1.31666m - 0.23888n + 1.03333$

10. $NI(OG_{m\times n}) = S_xJD_xD_y\,f(x,y)\big|_{x=y=1} = 27m^2 + \frac{589}{24}m - \frac{923}{24}n + \frac{457}{36}$

11. $S(OG_{m\times n}) = {S_x}^3 Q_{-2}\, J {D_x}^3 {D_y}^3\, f(x,y)\big|_{x=y=1}$

$$= \frac{129140163}{2048}m^2 + \frac{4866593}{256}m - \frac{262394303}{2048}n + \frac{241826917177}{4741632}$$

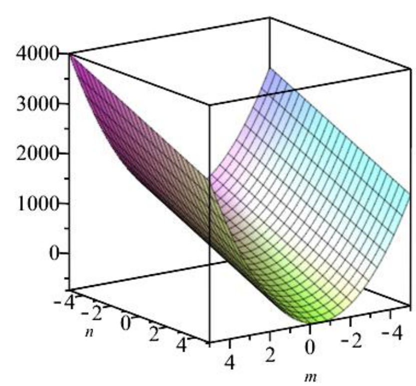
12. $NHM_1G_5(OG_{m\times n}) = \left({D_x}^2 + {D_y}^2 + 2D_xD_y\right)\left(f(x,y)\right)_{x=y=1} = 1944m^2 + 1288m - 3248n + 920$

13. $NHM_2G_5(OG_{m\times n}) = D_xD_y\left(D_xD_y\right)\left(f(x,y)\right)_{x=y=1} = 39366m^2 + 14088m - 77766n + 28536$

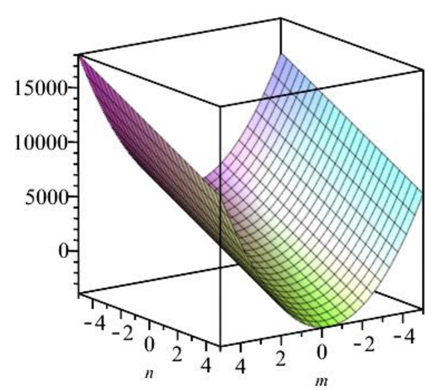
14. $NAG_5(OG_{m\times n}) = \frac{1}{2}{S_x}^{\frac{1}{2}}{S_y}^{\frac{1}{2}}\left(D_x + D_y\right)\left(f(x,y)\right)_{x=y=1} = 6m^2 + 2m - 12n + \frac{24m+24n-48}{\sqrt{35}} + \frac{256m+256n-512}{\sqrt{63}} + 8 + \frac{36}{\sqrt{20}}.$

15. $NGA_5(OG_{m\times n}) = 2S_xJ{D_x}^{\frac{1}{2}}{D_y}^{\frac{1}{2}}\left(f(x,y)\right)_{x=y=1} = 6m^2 + 2m - 12n + \frac{2\sqrt{35}(m+n-2)}{3} + \frac{\sqrt{72}(m+n-2)}{4} + 8 + \frac{16\sqrt{20}}{9}.$

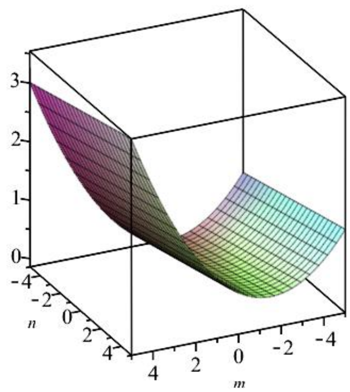
Some neighborhood topological indices of the Octa-graphene structure of $OG_{m\times n}$ are depicted in Figure 4.



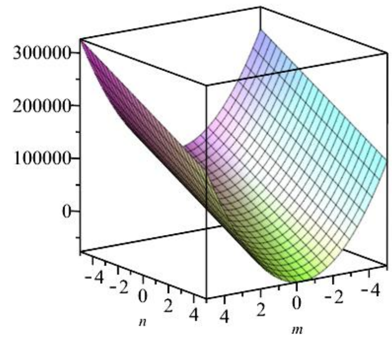
$NM_1(OG_{m\times n})$



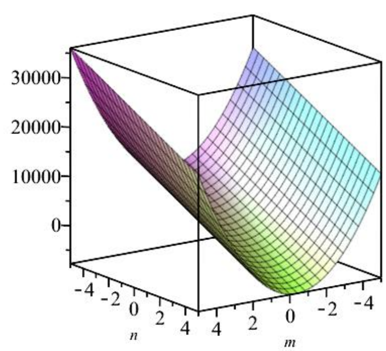
$NM_2(OG_{m\times n})$



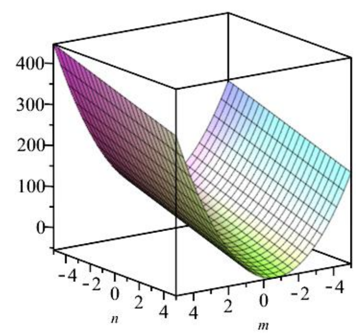
$NmM_2(OG_{m\times n})$



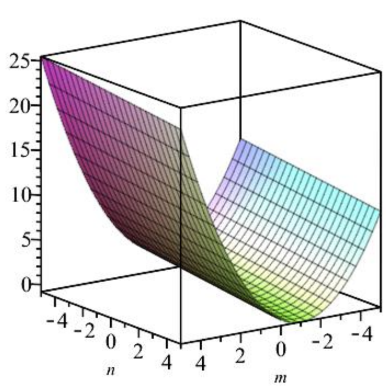
$ND_3(OG_{m\times n})$



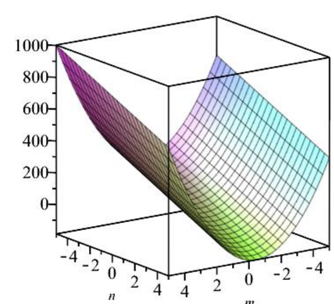
$NF(OG_{m\times n})$



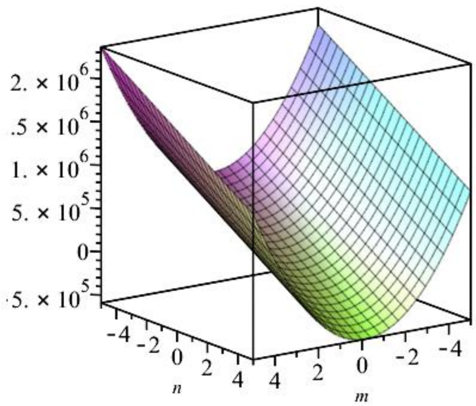
$ND_5(OG_{m\times n})$



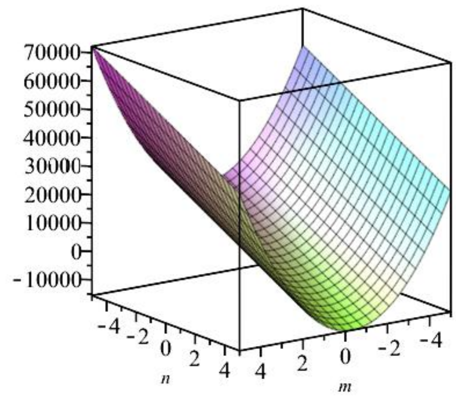
$NH(OG_{m\times n})$



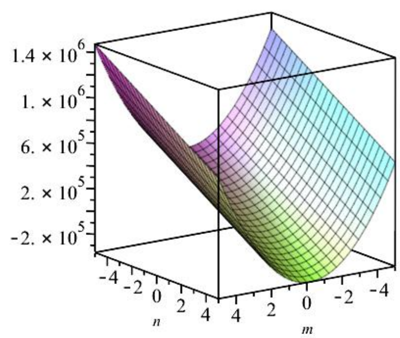
$NI(OG_{m\times n})$



$S(OG_{m\times n})$



$NHM_1G_5(OG_{m\times n})$



$NHM_2G_5(OG_{m\times n})$

Figure 4. Neighborhood topological indices of $OG_{m\times n}$

Conclusion

Carbon-based nanosheets come in a variety of shapes and sizes, making them incredibly versatile materials with applications in many different fields. To truly understand these materials, we need to analyze their underlying structure. In this study, we focused on Octa-graphene nanosheet and used a specific mathematical technique called the neighborhood *M*-polynomial to calculate various neighborhood topological indices. By visualizing these indices, we gained valuable insights into the structure and potential properties of Octa-graphene. These results can be useful in gaining deeper insights into the structural features of the Octa-graphene.

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