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石墨烯的一些多项式和基于度的拓扑指数

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摘要：图 G 的拓扑指数是与 G 相关的数值参数，其刻画了图的拓扑并在图同构下保持不变. 而化学化合物的性质和拓扑指数是相关的. 因此，计算了石墨烯的第 1 类和第 2 类萨格勒布多项式，以及遗忘多项式，同时还得到石墨烯的第 1 类和第 2 类乘法萨格勒布指数和遗忘指数.

关键词：理论化学；石墨烯；萨格勒布多项式；萨格勒布指数
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Some Polynomials and Degree-based Topological Indices of Graphene

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Abstract：The topological index of graph G is a numerical parameter related to G，which characterizes its topology and is preserved under isomorphism of graphs. Properties of the chemical compounds and topological indices are correlated. So we compute the first and second Zagreb polynomials and forgotten polynomial of graphene. At the same time，we get the first and second multiple Zagreb indices and forgotten index of grapheme.
Key words：theoretical chemistry；grapheme；Zagreb polynomial；Zagreb index

1　Basic Knowledge

Chemical reaction network theory is an area of applied mathematics that attempts to model the behavior of real world chemical systems. Since its foundation in the 1960s，it has attracted a growing research community，mainly due to its applications in biochemistry and theoretical chemistry. It has also attracted interest from pure mathematicians due to the interesting problems that arise from the mathematical patterns in structures of material.

Cheminformatics is an emerging field in which quantitative structure-activity（QSAR）and Structure-property（QSPR）relationships predict the biological activities and properties of nanomaterial. In these studies，some physcio-chemical properties and topological indices are usd to predict bioactivity of the chemical compounds[1-5].

The branch of chemistry which deals with the chemical structures with the help of mathematical tools is called mathematical chemistry. Chemical graph theory is the branch of mathematical chemistry that applies graph theory to

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mathematical modeling of chemical phenomena. In chemical graph theory, a molecular graph is a simple graph (having no loops and multiple edges) in which atoms and chemical bonds between them are represented by vertices and edges respectively. A graph G with vertex set $V(G)$ and edge set $E(G)$ is connected if there exists a connection between any pair of vertices in G. The distance between two vertices u and v is denoted as $d(u, v)$ and is the length of shortest path between u and v in graph G. The number of vertices of G, adjacent to a given vertex v, is the "degree" of this vertex and will be denoted by dv. For details on basics of graph theory, any standard text such as[6] can be of great help.

The first and the second Zagreb indices (cf.[7]) are defined as

$$M_1(G,x) = \sum_{uv \in E(G)} x^{[d(u)+d(v)]},$$

$$M_2(G,x) = \sum_{uv \in E(G)} x^{[d(u)d(v)]}.$$

The multiplicative version of the first and second Zagreb indices were first defined by Ghorbani and Azimi[8] as

$$PM_1(G) = \prod_{uv \in E(G)} [d(u)+d(v)],$$

$$PM_2(G) = \prod_{uv \in E(G)} [d(u)d(v)].$$

And Recently in 2015 Furtula and Gutman[9] introduced another topological index called forgotten index or F-index

$$F(G) = \sum_{uv \in E(G)} [d(u)^2 + d(v)^2].$$

The forgotten polynomial is defined as

$$F(G,x) = \sum_{uv \in E(G)} x^{[d(u)^2+d(v)^2]}.$$

Graphene is an atomic scale honeycomb lattice made of carbon atoms. Graphene is 200 times stronger than steel, one million times thinner than a human hair, and world's most conductive material. So it has captured the attention of scientists, researchers, and industrialists worldwide. It is one of the most promising nanomaterials because of its unique combination of superb properties, which opens a way for its exploitation in a wide spectrum of applications ranging from electronics to optics, sensors, and biodevices. Also it is the most effective material for electromagnetic interference (EMI) shielding. Now we focus on computation of topological indices of Graphene. In Figure 1, the molecular graph of Graphene is shown.

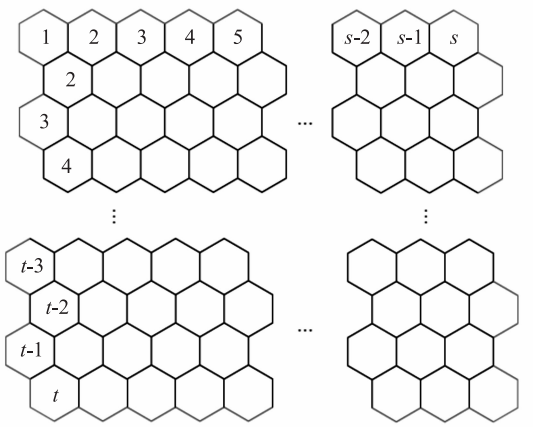

Figure 1　Molecular graph of graphene

2　Main Results and Proofs

In this paper we compute Zagreb polynomials, forgotten polynomial, multiple Zagreb indices and forgotten index of graphene. For details about topological indices and applications we refer[10-12] and references therein.

Theorem 1 Let G be molecular graph of graphene having t rows of Benzene rings with s Benzene ring in each row. Then the first Zagreb polynomial is

$$M_1(G,x) = (t+4)x^4 + (4s+2t-4)x^5 + (3ts-2s-t-1)x^6.$$

Proof Let G be molecular graph of grapheme (see Figure 1), then the edges of graphene are divided into three types:

$$E_{\{2,2\}}(G) = \{uv \in E(G) : d(u) = d(v) = 2\};$$
$$E_{\{2,3\}}(G) = \{uv \in E(G) : d(u) = 2, d(v) = 3\};$$
$$E_{\{3,3\}}(G) = \{uv \in E(G) : d(u) = d(v) = 3\}.$$

Such that $|E_{\{2,2\}}| = t+4, |E_{\{2,3\}}| = 4s+2t-4,$

and $|E_{\{3,3\}}| = 3ts-2s-t-1.$

Now from the definition, the first Zagreb polynomial of G is

$$M_1(G,x) = \sum_{uv \in E(G)} x^{[d(u)+d(v)]} = |E_{\{2,2\}}|x^{2+2} + |E_{\{2,3\}}|x^{2+3} + |E_{\{3,3\}}|x^{3+3}$$
$$= (t+4)x^4 + (4s+2t-4)x^5 + (3ts-2s-t-1)x^6.$$

Some plots of the first Zagreb polynomial of graph structure described in Theorem 1 can refer to Figure 2.

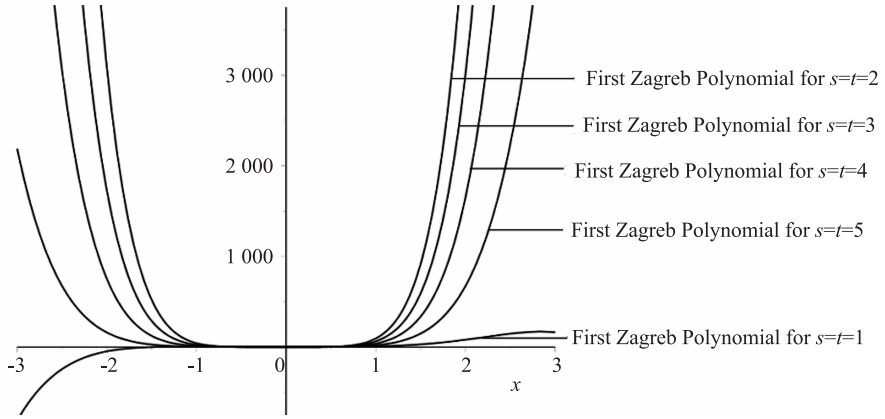

Figure 2 Plot of first Zagreb polynomial

Theorem 2 Let G be molecular graph of graphene with t rows of Benzene rings with s Benzene ring in each row. Then the second Zagreb index is.

$$M_2(G,x) = (t+4)x^4 + (4s+2t-4)x^6 + (3ts-2s-t-1)x^9.$$

Proof From the definition of second Zagreb polynomial, we have

$$M_2(G,x) = \sum_{uv \in E(G)} x^{[d(u)\times d(v)]} = |E_{\{2,2\}}|x^{2\times 2} + |E_{\{2,3\}}|x^{2\times 3} + |E_{\{3,3\}}|x^{3\times 3}$$
$$= (t+4)x^4 + (4s+2t-4)x^6 + (3ts-2s-t-1)x^9.$$

Figure 3 below shows some plots of the second Zagreb polynomial of graph structure described in Theorem 2.

Theorem 3 Let G be molecular graph of graphene having t rows of Benzene rings with s Benzene ring in each row. Then the forgotten polynomial is

$$F(G,x) = (t+4)x^8 + (4s+2t-4)x^{13} + (3ts-2s-t-1)x^{18}.$$

Proof Form the definition of forgotten polynomial, we infer

$$F(G,x) = \sum_{uv \in E(G)} x^{[d(u)^2+d(v)^2]} = |E_{\{2,2\}}|x^{[(2)^2+(2)^2]} + |E_{\{2,3\}}|x^{[(2)^2+(3)^2]} + |E_{\{3,3\}}|x^{[(3)^2+(3)^2]}$$
$$= (t+4)x^8 + (4s+2t-4)x^{13} + (3ts-2s-t-1)x^{18}.$$

Figure 4 below manifests several plots of the forgotten polynomial of graph structure described in Theorem 3.

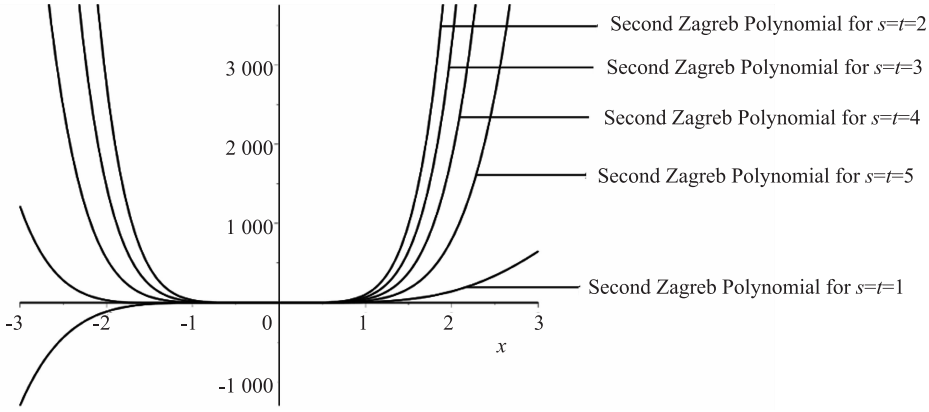

Figure 3　Plot of second Zagreb polynomial

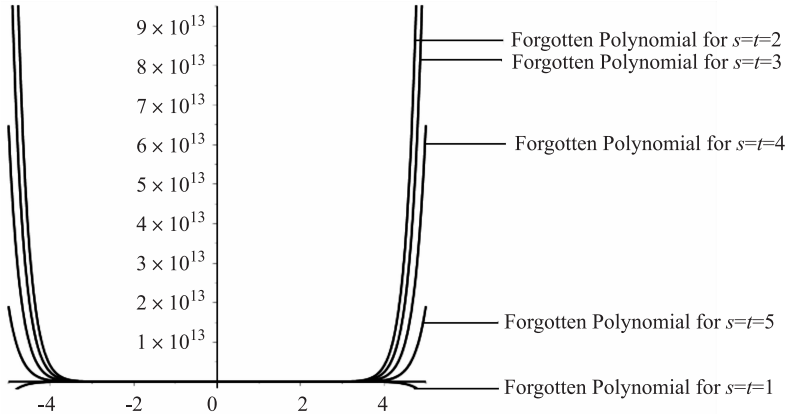

Figure 4　Plot of forgotten polynomial

Theorem 4　Let G be molecular graph of graphene having t rows of Benzene rings with s Benzene ring in each row. Then the first multiple Zagreb index is

$$PM_1(G) = (4)^{t+4} \times (5)^{4s+2t-4} \times (6)^{3ts-2s-t-1}.$$

Proof　From the definition of first multiple Zagreb index

$$\begin{aligned} PM_1(G) &= \prod_{uv \in E(G)} [d(u) + d(v)] \\ &= [d(u) + d(v)]^{|E_{2,2}|} \times [d(u) + d(v)]^{|E_{2,3}|} \times [d(u) + d(v)]^{|E_{3,3}|} \\ &= (2+2)^{t+4} \times (2+3)^{4s+2t-4} \times (3+3)^{3ts-2s-t-1} \\ &= (4)^{t+4} \times (5)^{4s+2t-4} \times (6)^{3ts-2s-t-1}. \end{aligned}$$

Also, Figure 5 presents some plots of the first multiple Zagreb index of graph structure described in Theorem 4.

Theorem 5　Let G be molecular graph of grapheme graphene having t rows of Benzene rings with s Benzene ring in each row. Then the second multiple Zagreb polynomial is

$$PM_2(G) = (4)^{t+4} \times (6)^{4s+2t-4} \times (9)^{3ts-2s-t-1}.$$

Proof　From the definition of second multiple Zagreb index, we deduce

$$\begin{aligned} PM_2(G) &= \prod_{uv \in E(G)} [d(u) \times d(v)] \\ &= [d(u) \times d(v)]^{|E_{2,2}|} \times [d(u) \times d(v)]^{|E_{2,3}|} \times [d(u) \times d(v)]^{|E_{3,3}|} \\ &= (2 \times 2)^{t+4} \times (2 \times 3)^{4s+2t-4} \times (3 \times 3)^{3ts-2s-t-1} \\ &= (4)^{t+4} \times (6)^{4s+2t-4} \times (9)^{3ts-2s-t-1}. \end{aligned}$$

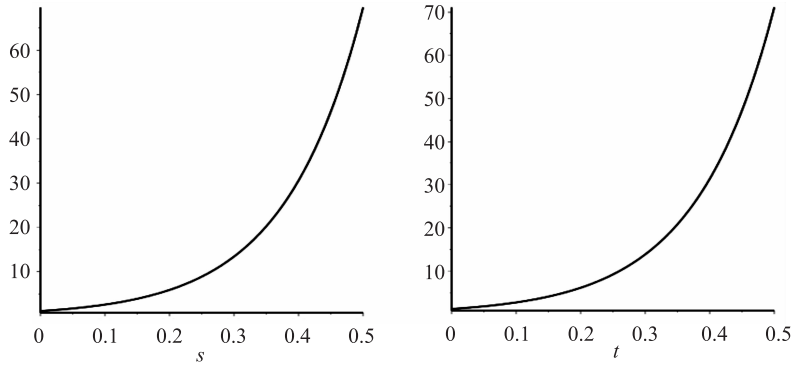

Figure 5 Plot of first multiplicative Zagreb index (for t=1 left and for s=1 right)

Again, Figure 6 presents some plots of the second multiple Zagreb index of graph structure described in Theorem 5.

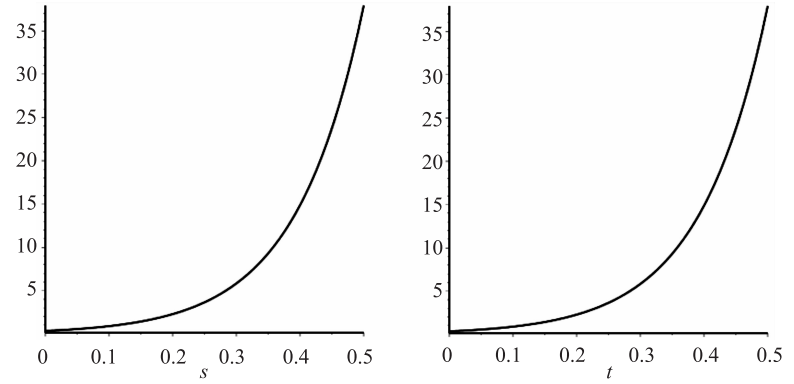

Figure 6 Plot of second multiplicative Zagreb index (for t=1 left and for s=1 right)

Theorem 6 Let G be molecular graph of graphene having t rows of Benzene rings with s Benzene ring in each row. Then the forgotten index is

$$F(G) = 54ts + 16t + 16s - 38.$$

Proof From the definition of forgotten index, we get

$$\begin{aligned} F(G) &= \sum_{uv \in E(G)} [d(u)^2 + d(v)^2] \\ &= |E_{\{2,2\}}|[2^2 + 2^2] + |E_{\{2,3\}}|[2^2 + 3^2] + |E_{\{3,3\}}|[3^2 + 3^2] \\ &= 8(t+4) + 13(4s + 2t - 4) + 18(3ts - 2s - t - 1) \\ &= 54ts + 16t + 16s - 38. \end{aligned}$$

Finally, in Figure 7 we show some plots of the forgotten index of graph structure described in Theorem 6.

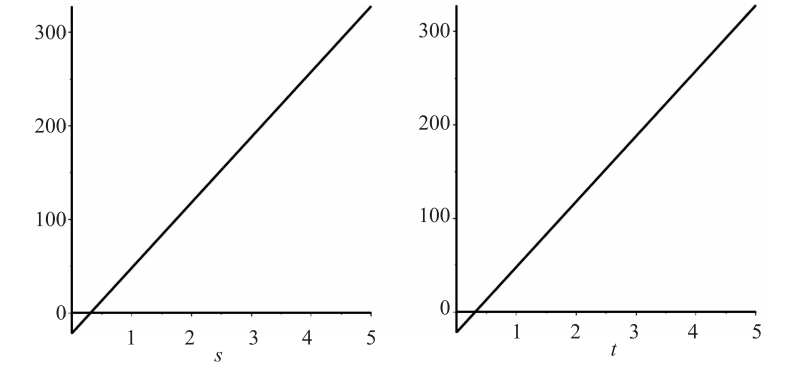

Figure 7 Plot of forgotten index (for t=1 left and for s=1 right)

3 Conculusion

In this report, we computed some degree-based topological indices for graphene. We aslo computed some algebric polynomials that describe molecular topology of graphene. Moreover we ploted our results to see the dependence on the involved structural paramenter.

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