Hindawi
Journal of Chemistry
Volume 2022, Article ID 7311404, 11 pages
https://doi.org/10.1155/2022/7311404

Research Article

A Survey on Generalized Topological Indices for Silicon Carbide Structure

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Received 24 January 2022; Revised 11 March 2022; Accepted 4 May 2022; Published 2 June 2022

Academic Editor: Hani Shaker

The application of graphs in chemical and molecular structures has exponentially increased during the last few years. Topological indices facilitate the collection of beneficial information and provide an approach to understanding the properties of chemical structure by providing information about algebraic graphs. Let G be a graph with u-vertices and $\Omega(u)$ be the degree of u^{th} vertex. In this manuscript, we compute Zagreb index (ZI), first, and second, Hyper F-indices and sum and product connectivity of F-index of silicon carbides, namely, $SiC_4 - I[r, s]$ and $SiC_4 - II[r, s]$.

1. Introduction

Graph theory deals with the study of the mathematical structures of chemical compounds. Chemical graph theory has a wide range of applications, including mathematical chemistry, quantization of structure-activity relationships (QSARs), and research into closeness diversity in subatomic libraries [1].

A graph is composed of vertices (nodes or points) that are connected by edges (arcs or lines). A graph may be directed (proper direction from one vertex to another vertex within an edge) or undirected (no difference between vertices and edges). A molecular graph is considered simple and connected, which deals with bonds and atoms by displaying their edges and vertices. The number of vertices that are connected to the fixed vertex is known as the degree of a vertex. In a simple graph, no multiple edges or loops exist. For example, the idea of valence electrons in chemistry is very close to the degree of vertices in graph theory. For more information about graph theory, see [2].

Chemical graph theory has wide application in chemistry and drug design. Graph theory is a very fascinating and unique subject in discrete mathematics and has many applications in real life [3–6]. In this paper, V denotes the set of vertices and E belongs to the set of edges. Topological indices can also be known as connectivity indices and are molecular descriptors that are computed using molecular graphs of chemical compounds in chemical graph theory and mathematical chemistry [7–10]. The topological indices play an important role in theoretical chemistry. Many topological indices are based upon the degree of a vertex in a chemical graph. Topological indices are used to understand and develop the mathematical properties of real-world network models.

The idea of topological indices was introduced by Wiener [11] when he was approximating the boiling points of alkanes in 1947. He introduced the first topological index,

namely the Wiener index. The most commonly used topological indices are the Wiener, Randic, and Zagreb indices [12–14]. The number of topological indices defined so far is more than 140, but these are insufficient for understanding the physicochemical properties of molecules. Chemical structure and biological activity of molecules are correlated when using topological indices to develop quantitative structure-activity relationships (QSARs) [15–18].

In 1891, Edward Goodrich Acheson prepared silicon carbide artificially from silica and carbon while he was working on the production of artificial diamonds. As a nontoxic and inexpensive compound with unlimited resources, silicon has superior properties over other semiconductors.

In computer and electronic devices, silicon is an extensively used compound as a semiconductor and it was assumed to be one of the hardest materials till 1929. SiC has a covalent bond between silicon and carbon. Silicon carbide has a very short bond length and a very high melting point. It has strong covalent bonds. It also has extremely high mechanical and chemical stability [19, 20]. Due to these properties, it is the backbone of almost all modern electronic gadgets. The most decent 2D structure of a silicon carbide monolayer with different stoichiometric parts was predicted in references [21, 22]. It is also used in optics because of its high mechanical quality and matchless electronic conductivity.

A large number of articles have been published on the importance of topological indices. Mahboob et al. have proposed many papers on the topological indices of silicon structure. In their article, they used many approaches to find the physical and chemical properties of different isomers of silicon carbide [23–25].

2. Preliminaries

Suppose G be a simple graph with $V(G)$ and $E(G)$ as sets of nodes and links, respectively. If two nodes u and v of a graph G are connected by a line said to be an edge denoted by uv or (u, v). The number of first neighbors vertices of vertex $u\epsilon$ V (G) is its degree and denoted by $\Omega(u)$.

(1) A new index namely the generalization of the Zagreb index [26] is defined as

$$M_{\alpha,\beta}(G) = \sum_{uv\epsilon E(G)} \frac{(\Omega(u) \times \Omega(v))^{\alpha}}{(\Omega(u) + \Omega(v))^{\beta}}, \tag{1}$$

where α and β are arbitrary real numbers.

(2) The same index was determined under the name, second Gourava index [27], obtained as a special case of generalized Zagreb index $M_{a,b}$ [28].

$$M_{a,b} = M_{a,b}(G) = \sum_{uv\epsilon E(G)} \left[\Omega(u)^{a} \times \Omega(v)^{b} + \Omega(u)^{a} \times \Omega(v)^{b}\right]. \tag{2}$$

(3) The concept of the F-index was proposed byFurtula and Gutman [29]. Ghebadi and Gborbani [30] invented the notion of Hyper F-index/first Hyper F-index as

$$HF_1(G) = \sum_{uv\epsilon E(G)} \left(\Omega(u)^2 + \Omega(v)^2\right)^2. \tag{3}$$

(4) Kulli [31] discussed the Hyper F-indices. The second Hyper Forgotten index of the graph G is mathematically stated as

$$HF_2(G) = \sum_{uv\epsilon E(G)} \left(\Omega(u)^2 \times \Omega(v)^2\right)^2. \tag{4}$$

(5) The notion of sum and product connectivity F-index of a graph G is computed as

$$SF(G) = \sum_{uv\epsilon E(G)} \frac{1}{\sqrt{\Omega(u)^2 + \Omega(v)^2}}, \tag{5}$$

$$PF(G) = \sum_{uv\epsilon E(G)} \frac{1}{\sqrt{\Omega(u)^2 \times \Omega(v)^2}}. \tag{6}$$

Wang et al. [32] applied these indices to the silicon structures to understand the characteristics of these compounds.

2.1. Various Methods. By combinatorial and computing rules (a method to count possible outcomes in a symmetrical structure), edge partition (a division of edges according to different degrees), vertex partition, graph-theoretical tools, degree counting method, and the sum of the degree of neighbors method. MATLAB and Maple are mathematical software used for mathematical calculations and plotting results (plotting).

3. Mathematical Modeling

The topological index is a numerical function that tells us about the different properties of chemical structures without any laboratory experiment. The term "topological index" was introduced by Harry Wiener in 1947 when he was estimating the boiling of paraffin [11]. The W-index is a distance-based topological index named "path number" by Wiener. It is defined as

$$W = \sum_{u=1}^{s} \sum_{v=1}^{s} (\Omega)_{uv}. \tag{7}$$

Example 1. Linear Alkanes.

The correlation coefficient between the Wiener index and some alkanes is $r = 0.87039$, so we can investigate the boiling points of these alkanes by using the Wiener index. If the values of r are near zero, then there is no relation between physical property and a topological index.

Example 2. Octane Isomers.

In 1972, Gutman and Trinajstic studied that the total pi-electron energy (E) depends upon the sum of squares of the vertex degrees of the molecular graph (later named the first

Table 1: The correlation coefficient between BP and W-index.

Name of alkane	Boiling point in celsius	Wiener index
Methane	−162	0
Ethane	−89	1
Propane	−42	4
n-Butane	0	10
n-Pentane	36	20
n-Hexane	69	35
n-Heptane	98	56

Zagreb index) and thus provides a measure of the branching of the carbon-atom skeleton [12].

$$M_1(G) = \sum_{v\varepsilon V(G)} (\Omega v)^2 = \sum_{uv\varepsilon E(G)} (\Omega u + \Omega v). \quad (8)$$

The sum of cubes of the degree of vertices also has a relation with pi-electron energy. However, at that time, it was ignored. In 2015, Furtula and Gutman show its relation with pi-electron energy and give a name to this index "Forgotten index" [29]. The forgotten index significantly enhances the physiochemical applicability of the first Zagreb index.

$$F(G) = \sum_{v\varepsilon V(G)} (\Omega v)^3 = \sum_{uv\varepsilon E(G)} \left(\Omega u^2 + \Omega v^2\right). \quad (9)$$

A set of data relating to octane consists of the following values: boiling point, melting point, heat capacities, entropy, density, the heat of vaporization, enthalpy of formation, motor octane number, molar refraction, acentric factor, total surface area, octanol-water partition coefficient, and molar volume. We correlated the F-index with each of these properties and compared the results with those obtained from using the first Zagreb index. The F-index is found to be quite similar to M_1 in terms of its predictive ability. In the case of entropy and acentric factor, both M_1 and F yield correlation coefficients greater than $r = 0.95$. On the other hand, for other physicochemical properties, neither M_1 nor F is satisfactorily correlated.

Example 3. Asthma Drugs.

The forgotten index has a relation to both the 1st and 2nd Zagreb index. So, it is useful to find all those properties that can be determined by Zagreb indices. The correlation coefficient for the Asthma drugs is given in Table 1.

Silicon carbide is a very useful compound for automobile parts, electric systems, electronic circuits, astronomy, thin filament pyrometer, heating elements, jewelry, and steel production. So, the structure of silicon is very important. Topological indices help to understand the deep study of the structure of silicon.

We can find the boiling points, molar mass, enthalpy of formation, enthalpy of combustion, density, log p, melting point, flash point, and eccentric factor with the help of the correlation coefficient between the index and physical property as we have computed above for some alkanes in Table 2.

Table 2: The correlation coefficient for the Asthma drugs.

Index	Boiling Points	Enthalpy
M_1 (G)	0.97	0.963
M_2 (G)	0.966	0.959
F (G)	0.944	0.936
SC (G)	0.971	0.964

4. Structural Information about $SiC_4 - I[r, s]$

The 2D structure of silicon carbide $SiC_4 - I[r, s]$ is displayed, where carbon (C) atoms are brown and silicon (Si) atoms are blue.

The chemical graph (Figures 1(a) and 1(b), 2(a) and 2(b)) indicates how unit cells connect each other to get more columns and rows which enhance physical development of the structure SiC_4–$I[r, s]$ with different orders. The simple procedure of constructing chemical structures consists of increasing row length by connecting the unit cells in the "r" direction, while increasing row height by increasing the unit cells in the "s" direction. In Figure 1(a), the unit provides a basic building block of the structure while the complex molecular graph where "r" cells connected through a row and "s" rows in which every row consists of "r" cells has been shown (Figure. 1(b)). In Figures. 2(a) and 2(b), a single row or chain of unit cells with connection of two rows of the SiC_4–$I[r, s]$ is shown.Consequently, cardinality of nodes and links in SiC_4–$I[r, s]$ are $|V(SiC_4\text{–}I[r, s])| = 10rs$ and $|E(SiC_4\text{–}I[r, s])| = 15rs - 5r - 2s + 5$, respectively.

5. Fundamental Outcomes for Silicon Carbide $(SiC_4 - I[r, s])$

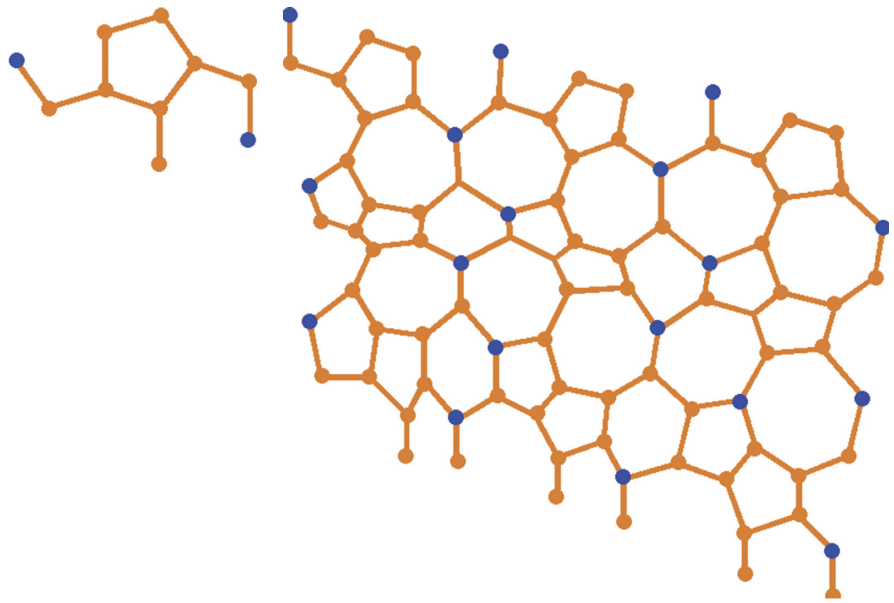
In this section, we calculate the fixed Tis, namely, the generalization of Z-indices, 1st and 2nd Hyper F-indices, the sum connectivity of F-indices, and the product connectivity of F-indices graph of SiC_4–$I[r, s]$.

In order to compute our indices, we use different order structures of SiC_4–$I[r, s]$.

Theorem 1. *Suppose* $(SiC_4 - I[r, s])$ *is an isomer of silicon carbides, then,*

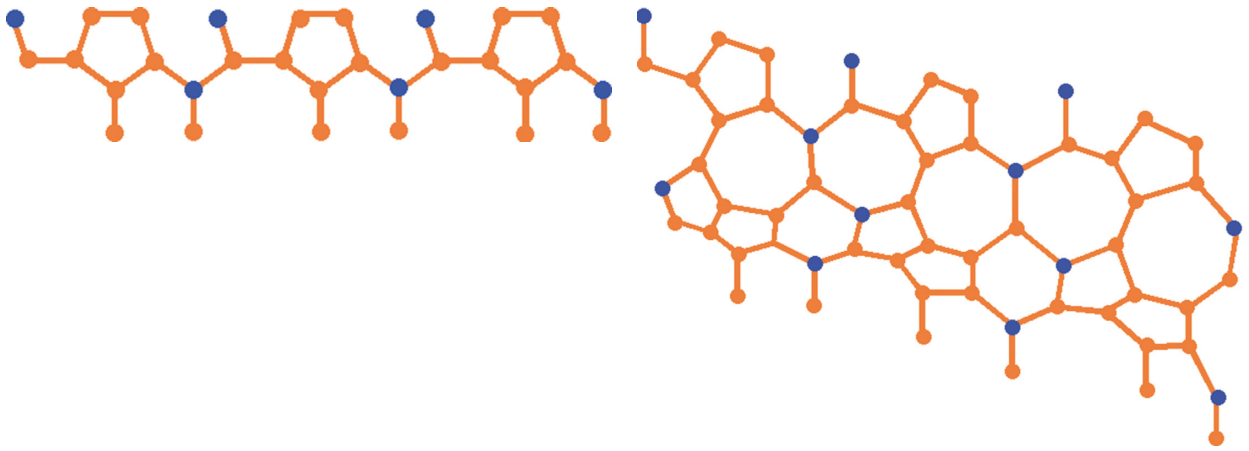
$$M_{\alpha,\beta}(SiC_4 - I[r, s]) = 9^{\alpha} \times \frac{15rs - 10r - 8s + 5}{6^{\beta}} + 6^{\alpha} \times \frac{2r + 4s - 2}{5^{\beta}} + 3^{\alpha} \times \frac{2r + 2}{4^{\beta}} + (r + 2s - 2) \times 4^{\alpha-\beta} + 2 \times \frac{2^{\alpha}}{3^{\beta}}, \quad (10a)$$

$$M_{a,b}(SiC_4 - I[r, s]) = (2r + 4s - 2) \times \left(2^a \times 3^b + 2^a \times 3^b\right) + (30rs - 20r - 16s + 10) \times 3^{a+b} + (2r + 4s - 4) \times 2^{a+b} + (2r - 2) \times \left(3^a \times 1^b + 3^a \times 1^b\right) + 2 \times 2^a + 2 \times 1^b. \quad (10b)$$



(a) (b)

Figure 1: (a) contains unit cell of $SiC_3 - I[r, s]$ and (b) contains $SiC_3 - I[3,3]$, $for\, r = 3,\ s = 3$.



(a) (b)

Figure 2: (a) contains a single row of silicon structure SiC_4–$I[3,1]$ with one row where $r = 3$and $s = 1$ and (b) contains two rows of silicon structure $SiC_4 - I[3,2]$ connected by red lines (edges).

Proof. Since silicon carbide SiC_4–$I[r, s]$ has total number of nodes $10rs$ and links $15rs - 5r - 32s + 5$, from Figures 1 and 2, we see nodes are divided into the following three partitions by degree partition of vertices.

$$V_1 = \left\{\frac{v\varepsilon V\left(SiC_4 - I[r,\ s]\right)}{\Omega(v) = 1}\right\},$$

$$V_2 = \left\{\frac{v\varepsilon V\left(SiC_4 - I[r,\ s]\right)}{\Omega(v) = 2}\right\}, \tag{11}$$

$$V_3 = \left\{\frac{v\varepsilon V\left(SiC_4 - I[r,\ s]\right)}{\Omega(v) = 3}\right\}.$$

The division of edges is as follows:

$$E1 = \left\{\frac{e = uv\varepsilon E\left(SiC_4 - I[r,s]\right)}{\Omega(u) = 2\ an\ d\ \Omega(v) = 1}\right\},$$

$$E2 = \left\{\frac{e = uv\varepsilon E\left(SiC_4 - I[r,s]\right)}{\Omega(u) = 3\ an\ d\ \Omega(v) = 1}\right\},$$

$$E_3 = \left\{\frac{e = uv\varepsilon\, E\left(SiC_4 - I[r,s]\right)}{\Omega(u) = 2\ an\ d\ \Omega(v) = 2}\right\}, \tag{12}$$

$$E_4 = \left\{\frac{e = uv\varepsilon\, E\left(SiC_4 - I[r,s]\right)}{\Omega(u) = 2\ an\ d\ \Omega(v) = 3}\right\},$$

$$E_5 = \left\{\frac{e = uv\varepsilon E\left(SiC_4 - I[r,s]\right)}{\Omega(u) = 3\ an\ d\ \Omega(v) = 3}\right\}.$$

In the graph of $SiC_4 - I[r, s]$, we compute $|E_1| = 2$, $|E_2| = 2r+2$, $|E_3| = r+2s-2$, $|E_4| = 2r+4s-2$, and $|E_5| = 15rs - 10r - 8s + 5$. The total numbers of edges with respect to their degree are given in Table 3.

Table 3: Edge division of $SiC_4 - I[r, s]$.

Edges $(\Omega(u), \Omega(v))$	Frequency
E_1 (1, 2)	2
E_2 (3, 1)	$2r+2$
E_3 (2, 2)	$r+2s-2$
E_4 (3, 2)	$2r+4s-2$
E_5 (3, 3)	$15rs-10r-8s+5$

Generalized Zagreb index $M_{\alpha,\beta}$ ($SiC_4 - I[r, s]$): the generalized Z-index for the silicon structure is determined as

$$\begin{aligned} M_{\alpha,\beta}(SiC_4 - I[r, s]) &= \sum_{uv\varepsilon E(G)} \frac{(\Omega(u) \times \Omega(v))^{\alpha}}{(\Omega(u) + \Omega(v))^{\beta}} \\ &= 2 \times \frac{(2 \times 1)^{\alpha}}{(2+1)^{\beta}} + (2r+2) \times \frac{(3 \times 1)^{\alpha}}{(3+1)^{\beta}} + (r+2s-2) \times \frac{(2 \times 2)^{\alpha}}{(2+2)^{\beta}} \\ &\quad + (2r+4s-2) \times \frac{(2 \times 3)^{\alpha}}{(2+3)^{\beta}} + (15rs - 10r - 8s + 5) \times \frac{(3 \times 3)^{\alpha}}{(3+3)^{\beta}} \\ &= \frac{9^{\alpha}}{6^{\beta}} \times (15rs - 10r - 8s + 5) + \frac{6^{\alpha}}{5^{\beta}} \times (2r + 4s - 2) + \frac{3^{\alpha}}{4^{\beta}} \times (2r+) \\ &\quad + (r + 2s - 2) \times 4^{\alpha-\beta} + 2 \times \frac{2^{\alpha}}{3^{\beta}}. \end{aligned} \tag{13}$$

Generalized Zagreb index $M_{r,s}(SiC_4 - I[r, s])$: by the statement of generalized Z-index of $SiC_4 - I[r, s]$, we have

$$M_{a,b} = M_{a,b}(SiC_4 - I[r, s]) = \sum_{uv\varepsilon E(G)} \left[\Omega(u)^a \times \Omega(v)^b + \Omega(u)^b \times \Omega(v)^a\right]$$

$$\begin{aligned} M_{a,b}(SiC_4 - I[r, s]) &= 2 \times \left(2^a \times 1^b + 2^b \times 1^a\right) + (2r+2) \times \left(3^a \times 1^b + 3^b \times 1^a\right) \\ &\quad + (r + 2s - 2) \times \left(2^a \times 2^b + 2^b \times 2^a\right) + (2r + 4s - 2) \times \left(2^r \times 3^s + 2^s \times 3^r\right) \\ &\quad + (15rs - 10r - 8s + 5) \times \left(3^a \times 3^b + 3^b \times 3^a\right) \\ M_{a,b} &= (2r + 4s - 2) \times \left(2^r \times 3^s + 2^s \times 3^r\right) + (30rs - 20r - 16s + 10) \times 3^{s+r} + (2r + 4s - 4) \\ &\quad \times 2^{a+b} + (2r+2) \times \left(3^a \times 1^b + 3^b \times 1^a\right) + 2 \times 2^a + 2 \times 1^b. \end{aligned} \tag{14}$$

Theorem 2. *Let $SiC_4 - I[r, s]$ be the silicon carbide, then, the 1st hyper F-index is as*

$HF_1(SiC_4 - I[r, s]) = 4860rs - 2638r - 1788s + 1004$,

$HF_2(SiC_4 - I[r, s]) = 98415rs - 62600r - 46792s + 29751$.

Proof. First hyper F-index HF_1 (SiC_4–$I[r, s]$): the cardinality of links and nodes are 10rs and 15rs – 5r – 2s + 5, respectively. By the definition of the first hyper F-index of SiC4–I [r, s], we have

$$\begin{aligned} HF_1(SiC_4 - I[r, s]) &= \sum_{uv\varepsilon E(G)} \left(\Omega(u)^2 + \Omega(v)^2\right)^2 \\ &= 2 \times \left(2^2 + 1^2\right)^2 + (2r-2) \times \left(3^2 + 1^2\right)^2 \\ &\quad + (r + 2s - 2) \times \left(2^2 + 2^2\right)^2 \\ &\quad + (2r + 4s - 2) \times \left(2^2 + 3^2\right)^2 \\ &\quad + (15rs - 10r - 8s + 5) \times \left(2^2 + 2^2\right)^2 \\ &= 4860rs - 2638r - 1788s + 1004. \end{aligned} \tag{15}$$

□

Second hyper F-index HF_2 (SiC_4–$I[r, s]$): from the statement of the second hyper F-index of $SiC_4 - I[r, s]$ as

$$\begin{aligned} HF_2\left(\left(SiC_4 - I[r, s]\right)\right) &= \sum_{uv\varepsilon E(G)} \left(\Omega(u)^2 \times \Omega(v)^2\right)^2 \\ &= 2 \times \left(2^2 \times 1^2\right)^2 + (2r - 2) \\ &\quad \times \left(3^2 \times 1^2\right)^2 + (r + 2s - 2) \\ &\quad \times \left(2^2 \times 2\right)^2 + (2rs + 4r - 2) \times \left(2^2 \times 3^2\right)^2 \\ &\quad + (15rs - 10r - 8s + 5) \times \left(3^2 \times 1^2\right)^2 \\ HF_2\left(\left(SiC_4 - I[r, s]\right)\right) &= 8415rs - 62600r \\ &\quad - 46792s + 2957, \end{aligned} \tag{16}$$

which is required result. □

Theorem 3. *Suppose we have silicon carbide of type SiC_4–I [r, s], then S-connectivity and P-connectivity F-indices are stated as*

$$\begin{aligned} SF\left(SiC_4 - I[r, s]\right) &= \sqrt{2} \times \left(\frac{5}{2}rs - \frac{5}{3}r - \frac{4}{3}s + \frac{5}{6}\right) \\ &\quad + \sqrt{13} \times \frac{(2r + 4s - 2)}{13} + \sqrt{2} \\ &\quad \times \left(\frac{r}{4} + \frac{s}{2} - \frac{1}{2}\right) + \sqrt{10} \times \left(\frac{r}{5} - \frac{1}{5}\right) + \sqrt{5} \times \frac{2}{5} \\ PF\left(SiC_4 - I[r, s]\right) &= \frac{5}{3}rs + \frac{5}{36}r + \frac{5}{18}s + \frac{1}{18}. \end{aligned} \tag{17}$$

Proof. Sum connectivity F-Index ($SiC_4 - I[r, s]$). We have computed the graph of $SiC_4 - I[r, s]$ has 10rs vertices and 15rs – 5r – 2s + 5 edges. So, the sum connectivity F-Index of $SiC_4 - I[r, s]$ is

$$\begin{aligned} SF(G) &= \sum_{uv\varepsilon E(G)} \frac{1}{\sqrt{\Omega(u)^2 + \Omega(v)^2}} \\ &= 2 \times \frac{1}{\sqrt{2^2 + 1^2}} + (2r - 2) \times \frac{1}{\sqrt{3^2 + 1^2}} + (r + 2s - 2) \\ &\quad \times \frac{1}{\sqrt{2^2 + 2^2}} + (2r + 4s - 2) \\ &\quad \times \frac{1}{\sqrt{2^2 + 3^2}} + (15rs - 10r - 8s + 5) \\ SF &= \sqrt{2} \times \left(\frac{5}{2}rs - \frac{5}{3}r - \frac{4}{3}s + \frac{5}{6}\right) + \sqrt{13}\ \frac{(2r + 4s - 2)}{13} \\ &\quad + \sqrt{2} \times \left(\frac{r}{4} + \frac{s}{2} - \frac{1}{2}\right) + \sqrt{10} \\ SF &= \sqrt{2} \times \left(\frac{5}{2}rs - \frac{5}{3}r - \frac{4}{3}s + \frac{5}{6}\right) + \sqrt{13}\ \frac{(2r + 4s - 2)}{13} \\ &\quad + \sqrt{2} \times \left(\frac{r}{4} + \frac{s}{2} - \frac{1}{2}\right) + \sqrt{10} \\ &\quad \times \left(\frac{r}{5} - \frac{1}{5}\right) + \sqrt{5} \times \frac{2}{5}. \end{aligned} \tag{18}$$

Product connectivity F-Index ($SiC_4 - I[r, s]$): P-connectivity F-Index for ($SiC_4 - I[r, s]$) is as follows:

$$\begin{aligned} PF(G) &= \sum_{uv\varepsilon E(G)} \frac{1}{\sqrt{\Omega(u)^2 \times \Omega(v)^2}} \\ &= 2 \times \frac{1}{\sqrt{2^2 \times 1^2}} + (2r - 2) \times \frac{1}{\sqrt{3^2 \times 1^2}} + (r + 2s - 2) \\ &\quad \times \frac{1}{\sqrt{2^2 \times 2^2}} + (2r + 4s - 2) \\ &\quad \times \frac{1}{\sqrt{2^2 \times 3^2}} + (15rs - 10r - 8s + 5) \\ PF &= \frac{5}{3}rs + \frac{5}{36}r + \frac{5}{18}s + \frac{1}{18}. \end{aligned} \tag{19}$$

(a) Graphical analysis for SiC_4–$I[r, s]$

We compare the topological indices graphically and check out their relations and properties. The graphical representation of SiC_4–$I[r, s]$ for $r = 1,2,3,\ldots, 10$ and $s = 1,2,3,\ldots, 10$ is given in Figures 3(a), 3(b), 3(c), and 3(d). □

6. Structural Information about SiC_4-*II*[*r*, *s*]

The 2D molecular structures of SiC_4–$II[r, s]$ are given in Figures 4 and 5, respectively.Chemical building blocks are built from unit cells, which are the basis of all chemical structures. If we attach the unit cells in "r" direction, then it increases the length of row, while if it increases unit cell in "s" style, then it enhances the number of rows. The quantity of nodes and links in SiC_4–$II[r, s]$ are represented as $|V(SiC_4 - II[r, s])| = 10rs$, $|E(SiC_4 - II[r, s])| = 15rs - 4r - 2s$.

7. Result for Silicon Carbon (SiC_4–*II*[*r*, *s*])

In this section, we compute the six TIs: the generalization of the Z-index, the first hyper F-index, the second hyper F-index, the S-connectivity, and the P-connectivity F-indices. TIs help to find the different properties of chemical products, such as melting and boiling points, the bond length of structure, bond strength, and nature of bonds. Chemical graph theory is the branch of graph theory in which the structures and shapes of chemicals are examined by graphs. These methods can save time and money on laboratory experiments. We can also predict the large silicon carbides.

Theorem 4. *Consider SiC_4–II[r, s] be the silicon carbide. Then, the generalization of the Z-index are given as follows:*

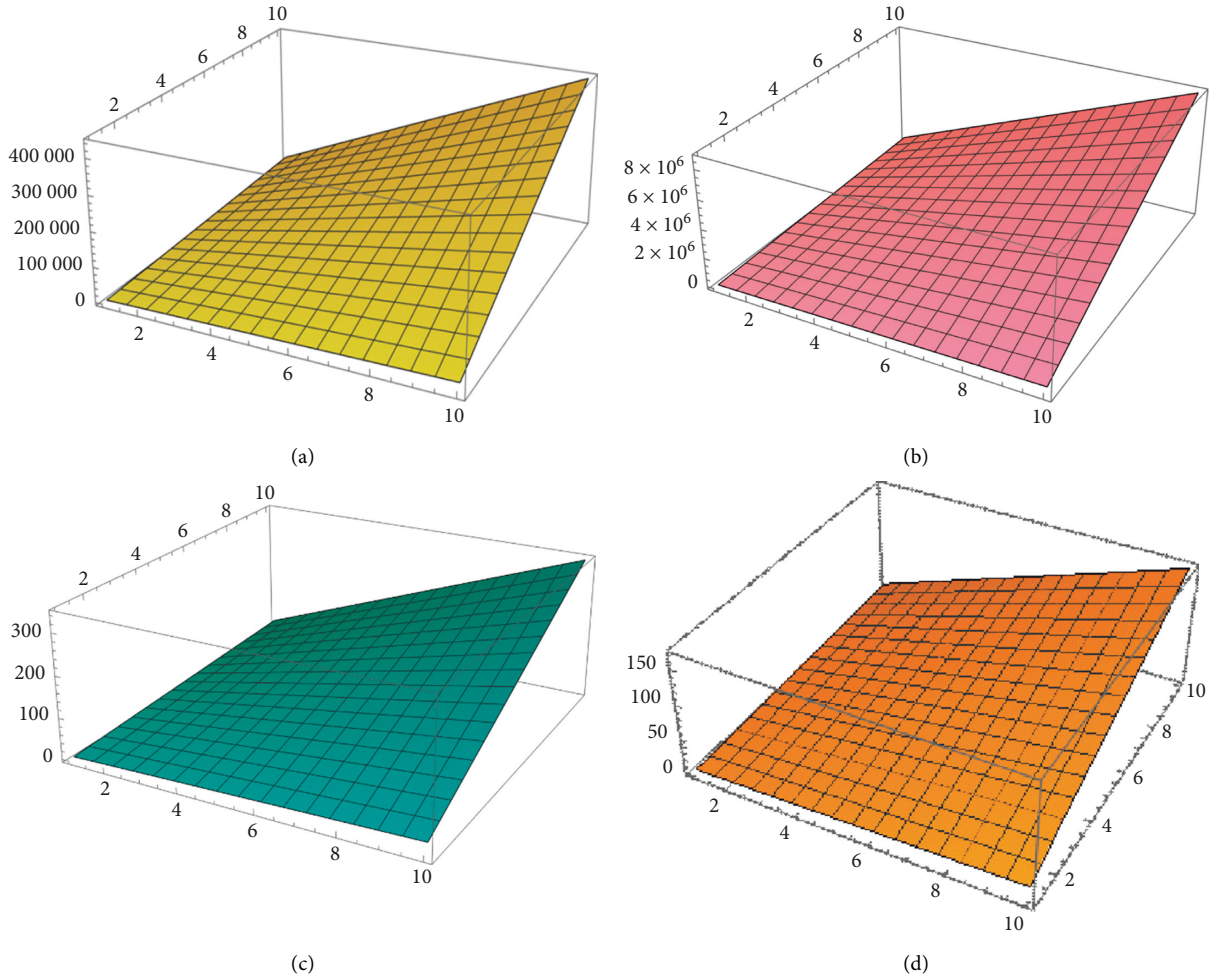


Figure 3: (a) First hyper F-index (HF1) SiC_4–$I[r, s]$. (b) Second hyper F-index (HF2) SiC_4–$I[r, s]$. (c) S-connectivity F-index $SiC_4 - I[r, s]$. (d) P-connectivity F-index SiC_4–$I[r, s]$.

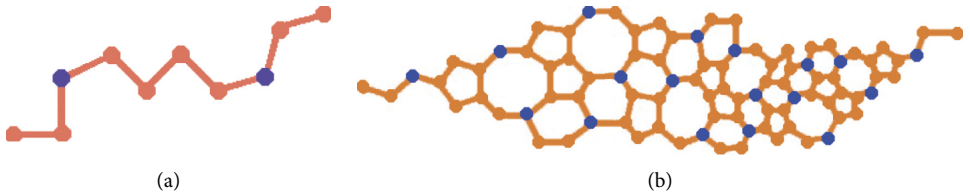


Figure 4: Two-dimensional structure of SiC_4–$II[r, s]$. (a) a unit cell of SiC_4–$II[r, s]$. (b) SiC_4–$II[r, s]$ for r = 3, s = 3.

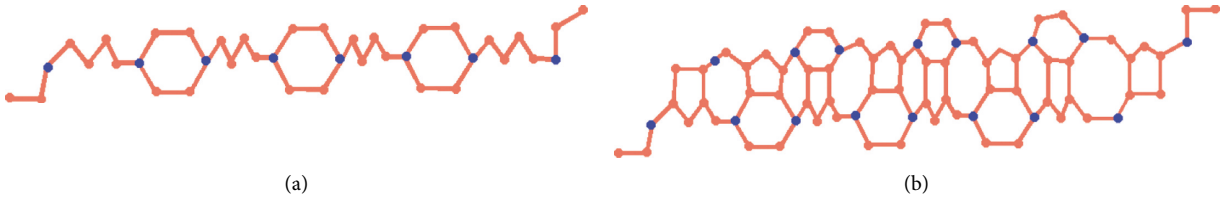


Figure 5: Two-dimensional structure of SiC_4–$II[r, s]$. (a) SiC_4–$II[r, s]$, one row with r = 4 and s = 1. (b) SiC_4–$II[r, s]$ for $r = 4$, $s = 2$.

$$M_{\alpha,\beta}(\mathrm{SiC}_4 - II[r,\ s]) = 9^{\alpha} \times \frac{15rs-18r-10s+\ 10}{6^{\beta}} + 6^{\alpha} \times \frac{12r+\ 8s-14}{5^{\beta}} + (2r+2) \times 4^{\alpha-\beta} + 2 \times \frac{2^{\alpha}}{3^{\beta}}$$

$$M_{r,s}(\mathrm{SiC}_4 - II[r,s]) = (12r+8s-14) \times \left(2^{a} \times 3^{b} + 2^{b} \times 3^{a}\right) + (30rs-36r-20s+20) \times 3^{a+b} + (4r+4) \times 2^{a+b} + 2 \times 1^{a} + 2 \times 2^{b}. \tag{20}$$

Proof. Suppose SiC_4–$II[r, s]$ be the silicon carbide and by the 2D graph, it contains total nodes 10rs and links 15rs – 4r – 2s. Then, by partitioning of SiC_4–$II[r,\ s]$ with respect to the degree vertices by using degree computing method, these partitions are

$$V_1 = \left\{\frac{v\varepsilon V(\mathrm{SiC}_4 - II[r,\ s])}{\Omega(v) = 1}\right\},$$

$$V_2 = \left\{\frac{v\varepsilon V(\mathrm{SiC}_4 - II[r,\ s])}{\Omega(v) = 2}\right\}, \tag{21}$$

$$V_3 = \left\{\frac{v\varepsilon V(\mathrm{SiC}_4 - II[r,\ s])}{\Omega(v) = 3}\right\}.$$

The edges division is defined as

$$E1 = \left\{\frac{e = E(\mathrm{SiC}_4 - II[r,\ s])}{\Omega(u) = 1\ an\ d\ \Omega(v) = 2}\right\},$$

$$E1 = \left\{\frac{e = E(SiC_4 - II[r,\ s])}{\Omega(u) = 1 \text{ and } \Omega(v) = 2}\right\},$$

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$$E1 = \left\{\frac{e = E(SiC_4 - II[r,\ s])}{\Omega(u) = 1 \text{ and } \Omega(v) = 2}\right\}.$$

The total numbers of edges with respect to their degree are given in Table 4.

The 2D molecular structure of SiC_4–$II[r,\ s]$ contains 4 types of degree base divisions denoted by E_1, E_2, E_3, and E_4, and the quantity of these edges is given in Table 4.

Generalized Zagreb index $M_{\alpha,\beta}(SiC_4$–$II[r,\ s])$ is as follows:

Table 4: Edge partition of $SiC_4 - II[r,\ s]$.

Edges ($\Omega(u)$, $\Omega(v)$)		Frequency
E_1	(1, 2)	2
E_2	(2, 2)	$2r+2$
E_3	(2, 3)	$12r+8s-14$
E_4	(3, 3)	$15rs-10s-18r+10$

$$M_{\alpha,\beta}(SiC_4 - II[r,s]) = \sum_{uv\varepsilon E(G)} \frac{(\Omega(u) \times \Omega(v))^{\alpha}}{(\Omega(u) + \Omega(v))^{\beta}}$$

$$M_{\alpha,\beta}(SiC_4 - II[r,s]) = 2 \times \frac{(1\times 2)^{\alpha}}{(1+2)^{\beta}} + (2r+2) \times \frac{(2\times 2)^{\alpha}}{(2+2)^{\beta}} + (12r+8s-2) \times \frac{(2\times 3)^{\alpha}}{(2+3)^{\beta}} + (15rs-10s-18r+10) \times \frac{(3\times 3)^{\alpha}}{(3+3)^{\beta}}$$

$$= 9^{\alpha} \times \frac{15rs-18r-10s+\ 10}{6^{\beta}} + 6^{\alpha} \times \frac{12r+\ 8s-14}{5^{\beta}} + (2r+2) \times 4^{\alpha-\beta} + 2 \times \frac{2^{\alpha}}{3^{\beta}}. \tag{23}$$

Generalization of Zagreb index $M_{a,b}(\mathrm{SiC}_4 - II[r,\ s])$ is as follows:

$$M_{a,b}(\mathrm{SiC}_4 - II[r,\ s]) = \sum_{uv\varepsilon E(G)} \left[\Omega(u)^{a} \times \Omega(v)^{b} + \Omega(u)^{b} \times \Omega(v)^{a}\right]$$

$$= 2 \times (1a \times 2b + 1b \times 2a) + (2r+2) \times (2a \times 2b + 2b \times 2a) + (21r+8s-14) \times (2a \times 3b + 2b \times 3a) + (15rs-10s-18r+10) \times (3a \times 3b + 3b \times 3a)$$

$$= (12r+8s-14) \times (2a \times 3b + 2b \times 3a) + (30rs-20s-36r+20) \times 3a + b + (4r+4) \times 2a + b + 2 \times 1a + 2 \times 2b. \tag{24}$$

□

Theorem 5. *Suppose SiC_4–$II[r,\ s]$ be the silicon carbide; then,*

$HF_1(SiC_4$–$II[r,\ s]) = 4860rs - 3676r - 1888s + 1052,$

$HF_2(SiC_4 - II[r,\ s]) = 98415rs - 10203r - 55242s + 48010.$

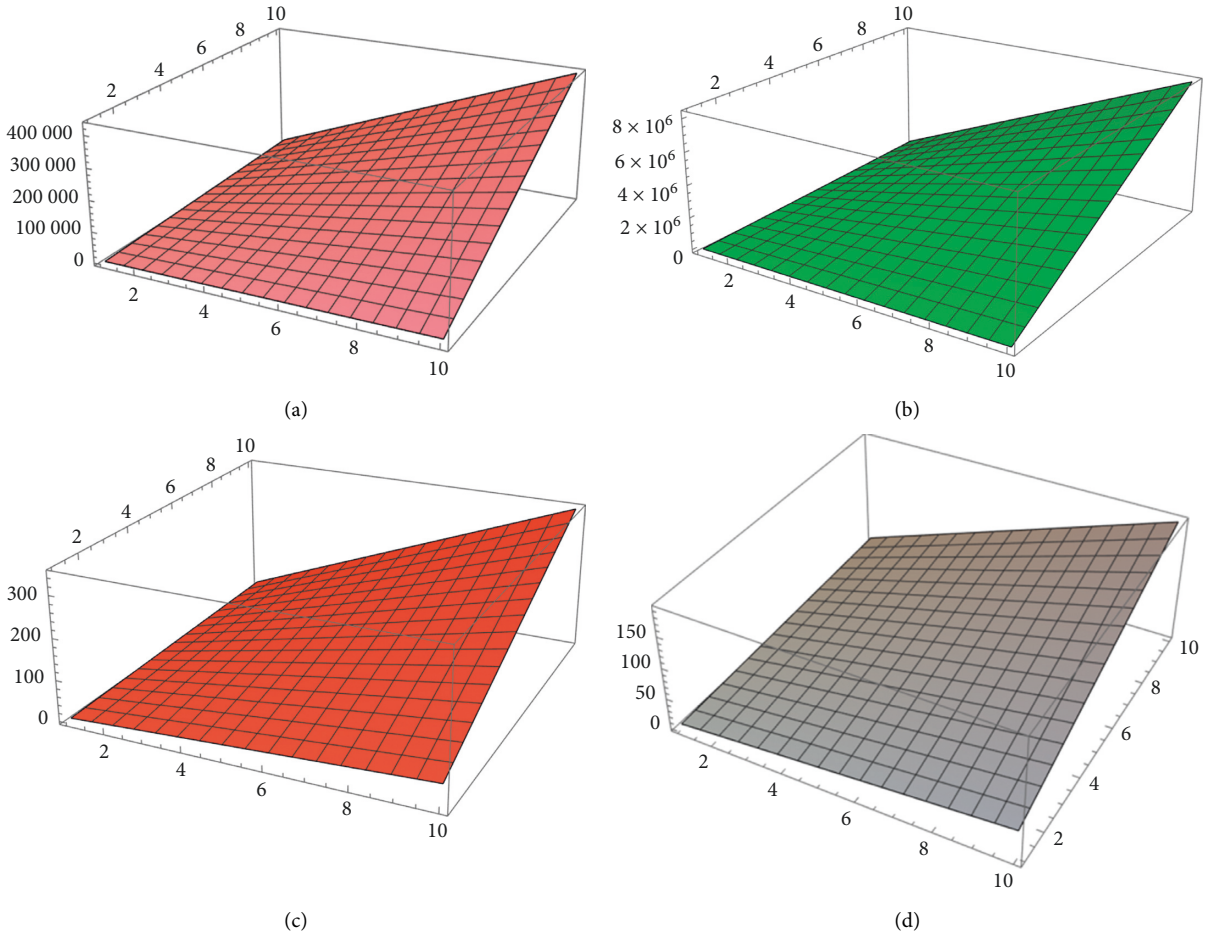

Figure 6: (a)HF_1 (SiC_4–$II[r, s]$), (b) HF_2 ($SiC_4 - II[r, s]$), (c) Sum connectivity F-index SiC_4–$II[r, s]$, and (d) Product Connectivity F-index $SiC_4 - II[r, s]$.

Proof. The graph of SiC_4–$II[r, s]$ contains 10rs nodes and 15rs – 4r – 2s links.

First Hyper F-index $HF_1(SiC_4$–$II[r, s])$: by the statement of 1st hyper F-index,

$$\begin{aligned} HF_1(SiC_4 - II[r, s]) &= \sum_{uv\varepsilon E(G)} \left(\Omega(u)^2 + \Omega(v)^2\right)^2 \\ &2 \times (12 + 22)2 + (2r + 2) \\ &\times (22 + 22) + (12r + 8s - 14) \\ &\times (22 + 32)2 \\ &+ (15rs - 10s - 18r + 10) \\ &\times (32 + 32)2 \\ &= 460rs - 3676r - 1888s + 1052. \end{aligned} \tag{25}$$

Second Hyper F-index $HF_2(SiC_4 - II[r, s])$: by the statement of 2nd hyper F-index,

$$\begin{aligned} HF_2((SiC_4 - II[r, s])) &= \sum_{uv\varepsilon E(G)} \left(\Omega(u)^2 \times \Omega(v)^2\right)^2 \\ &2 \times (12 \times 22)2 + (2r + 2) \\ &\times (22 \times 22) + (12r + 8s - 14) \\ &\times (22 \times 32)2 + (15rs - 10s \\ &- 18r + 10) \times (32 \times 32)2414 \\ &+ (15rs - 10s - 18r + 10) \\ &\times (32 \times 32)2 \\ HF_2(SiC_4 - II[r, s]) &= 98415rs - 102034r \\ &- 55242s + 48010, \end{aligned} \tag{26}$$

which is required result. □

Theorem 6. *SiC_4–II[r, s] is the silicon carbide that we are going to discuss. The sum connectivity and product connectivity indices are*

$$\begin{aligned}\mathrm{SF}\left(\mathrm{SiC}_4 - II[r,\ s]\right) &= \sqrt{2}\times\left(\frac{5}{2}rs - \frac{5}{3}r - 3s + \frac{5}{3}\right)\\ &\quad + \sqrt{13}\times\frac{(12r + 8s - 14)}{13}\\ &\quad + \sqrt{2}\times\left(\frac{r}{2} + \frac{1}{2}\right) + \sqrt{5}\times\frac{2}{5}\\ \mathrm{PF}\left(\mathrm{SiC}_4 - II[r, s]\right) &= \frac{5}{3}rs + \frac{5}{2}r + \frac{2}{9}s + \frac{5}{18}.\end{aligned} \tag{27}$$

Proof. By construction of the 2D molecular graph for silicon carbide. The graph of SiC_4–$II[r, s]$ contains 10rs vertices and 15rs – 4r – 2s edges.

Sum connectivity F-index $SF(SiC_4 - II[r, s])$ is as follows:

$$\mathrm{SF}(G) = \sum_{uv\varepsilon E(G)} \frac{1}{\sqrt{\Omega(u)^2 + \Omega(v)^2}}$$

$$\begin{aligned}\mathrm{SF}(\check{G}) &= 2\times\frac{1}{\sqrt{1^2 + 2^2}} + (2r + 2)\times\frac{1}{\sqrt{2^2 + 2^2}}\\ &\quad + (12r + 8s - 14)\times\frac{1}{\sqrt{2^2 + 3^2}}\\ &\quad + (15rs - 10s - 18r + 10)\times\frac{1}{\sqrt{3^2 + 3^2}}\end{aligned} \tag{28}$$

$$\begin{aligned}\mathrm{SF}(\check{G}) &= \sqrt{2}\times\left(\frac{5}{2}rs - \frac{5}{3}r - 3s + \frac{5}{3}\right) + \sqrt{13}\\ &\quad \times\frac{(12r + 8s - 14)}{13} + \sqrt{2}\times\left(\frac{r}{2} + \frac{1}{2}\right) + \sqrt{5}\times\frac{2}{5}.\end{aligned}$$

Product connectivity F-index $PF(SiC_4$–$II[r, s])$: using product connectivity F-Index for $SiC_4 - II[r, s]$, we have

$$\begin{aligned}\mathrm{PF}(G) &= \sum_{uv\varepsilon E(G)} \frac{1}{\sqrt{\Omega(u)^2 \times \Omega(v)^2}}\\ &= 2\times\frac{1}{\sqrt{1^2 \times 2^2}} + (2r + 2)\times\frac{1}{\sqrt{2^2 \times 2^2}}\\ &\quad + (12r + 8s - 14)\times\frac{1}{\sqrt{2^2 \times 3^2}}\\ &\quad + (15rs - 10s - 18r + 10)\times\frac{1}{\sqrt{3^2 \times 3^2}}\\ \mathrm{PF}(\check{G}) &= \frac{5}{3}rs + \frac{5}{2}r + \frac{2}{9}s + \frac{5}{18}.\end{aligned} \tag{29}$$

Graphical analysis for $(SiC_4$–$II[r, s])$: for a particular estimate in parameters "r" and "s" (see Figure 6(a), 6(b), 6(c), and 6(d)) yields the graphical representations of registered results about the generalization of first and second hyper F-indices and the sum and product connectivity F-indices of the silicon carbide SiC_4–$II[r, s]$. □

8. Conclusion

When some graph parameters are introduced in establishing appropriate bounds among some indices, it reveals a common challenge in the study of topological indices. The topological indices used in this article give us information about the different important properties of silicon carbide. Due to the great demand and usefulness of silicon carbide in the field of electronics, we try to explore different properties of this semiconductor with the help of mathematical formulae. We get a very good correlation of indices with the properties of silicon carbide. We estimated the behavior of silicon without performing any lab experiments. As a consequence effect of these topological indices, we compute, the generalization of Zagreb index, the first and second hyper F-index, and the sum and product connectivity F-index graphs of the silicon carbides SiC_4–I$[r, s]$ and SiC_4-II $[r, s]$.

Data Availability

No data were used in this manuscript.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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