Hindawi
Journal of Mathematics
Volume 2022, Article ID 5747464, 9 pages
https://doi.org/10.1155/2022/5747464

Research Article

Study of Ge-Sb-Te Superlattice Structure Based on Topological Descriptors

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Received 6 June 2022; Revised 15 July 2022; Accepted 9 September 2022; Published 3 October 2022

Academic Editor: Ljubisa Kocinac

Ge-Sb-Te superlattice is a new electronic material that is capable of storing nonvolatile phase-change memories with very low energy consumption. Topological descriptors are numerical values given to molecular structures that may be used to predict specific physical/chemical characteristics. In this work, we have investigated topological descriptors of the Ge-Sb-Te superlattice structure based on ev and ve-degree. We have calculated the Zagreb, geometric-arithmetic, Randic, and atom-bond connectivity indices of the Ge-Sb-Te superlattice structure using the ev- and ve-degrees. This kind of research may be beneficial for understanding the structure's chemical and biological activity.

1. Introduction

Chemical graph theory (CGT) utilizes topological indices to study the molecular topological characteristics of molecules. The values of a molecule's topological indices have a strong connection with certain chemical, biological, and physical characteristics of the molecule. This knowledge is utilized to simulate molecules' chemical and physical characteristics without experimental investigations. In 1947, Wiener developed the first distance-based topological index to model physical characteristics of alkanes [1], and Platt [2] proposed the degree-based topological index to model physical properties of alkanes. For details on the Zagreb indices and Platt index, we recommend the readers to [3]. Gutman and Trinajstic developed Zagreb indices more than forty years ago [4]. These topological indices (TIs) were suggested as carbon-atom-skeleton branching metrics in [5]. Recently, Chellali et al. presented two-degree new concepts: ve-degree and ev-degree in graph theory [6]. These novel-degree notions were developed by the authors regarding vertex-edge domination and edge-vertex domination parameters [7, 8]. Ev-degree and ve-degree topological indices were developed, and their fundamental mathematical characteristics were explored in [9].

An important article by Chellali et al. [6] proposed the concepts on ve- and ev-degrees in graphs. Certain basic mathematical features of these novel graph invariants had been investigated in terms of graph regularity and irregularity [6]. The chemical application of the total ev-degree (as well as the ve-degree) may be a fascinating topic to explore in light of chemistry and CGT, as well as other factors. Due to this approach, Ediz Suleyman [10] expanded these new degree concepts to CGT by establishing the ev- and ve-degree Zagreb and Randic indices. These indices have been demonstrated to have a stronger correlation with specific physicochemical properties of octanes than the Wiener, Zagreb, and Randic indices [10].

Huang et al. [11] computed the degree based indices for superlattice and shows their relation with heat of formation. It has been observed that the π-electron energy and strain energy can be predicted by using degree-based indices [12, 13]. Many researchers show that these degree-based indices are helpful in predicting the physical properties such as enthalpy, π-electron energy, enthalpy of vaporization, topological polar surface, acentric factor, molecular weight, and boiling point by developing QSPR [10, 14, 15]. In this paper, we compute ve-degree and ev-degree based indices for superlattices.

Let T be a graph with vertex set V and edge set E. The degree of a vertex v denoted by $\deg_v$ is the number of edges that are incident on a vertex v. The open neighbourhood $N(v)$ of vertex v is the collection of all neighbouring vertices to v. The closed neighbourhood of v, denoted by $N[v]$, is obtained by adding the vertex v to $N(v)$.

The first topological index by proposed by Weiner [1]. He named this index by Wiener index and is defined as follows [16]:

$$W(T) = \frac{1}{2} \sum_{u,v\in V(T)} d(u,v), \tag{1}$$

where $d(u,v)$ denoted the distance between the vertices u and v. Wiener computed paraffin's boiling point by calculating the total distance between all of its atoms (vertices). The interested readers may see [17, 18] for details on Wiener index. The first and second Zagreb indices were proposed by Gutman et al. [4] and are defined as

$$\begin{aligned} M_1(T) &= \sum_{uv\in E(T)} (\deg_u + \deg_v), \\ M_2(T) &= \sum_{uv\in E(T)} (\deg_u \times \deg_v). \end{aligned} \tag{2}$$

More details may on Zagreb indices can be found in [19, 20]. The Randic index [21] proposed by Milan Randic is defined as follows:

$$R(T) = \sum_{uv\in E(T)} (\deg_u \times \deg_v)^{-1/2}. \tag{3}$$

The readers may see [22, 23] for details on Randic index. Estrada et al. proposed ABC index [24] which is defined as

$$ABC(T) = \sum_{uv\in E(T)} \sqrt{\frac{\deg_u + \deg_v - 2}{\deg_u \times \deg_v}}. \tag{4}$$

More information regarding the ABC index may be found in [25, 26]. Vukievic and Furtula established the GA index [27]. The GA index is defined as:

$$GA(T) = \sum_{uv\in E(T)} \frac{2\sqrt{\deg_u \times \deg_v}}{\deg_u + \deg_v}. \tag{5}$$

For more details on GA index, see [28, 29]. Zhong proposed the harmonic index (H) [30] in 2012. The formula for H index is

Table 1: Ev-degrees and ve-degree-based indices.

	Notation	Formula
Ev-degree-based indices		
Randic index	R^{ev}	$\sum_{e\in E} \aleph_{ev}(e)^{-1/2}$
Zagreb index	M^{ev}	$\sum_{e\in E} \aleph_{ev}(e)^2$
Ve-degree-based indices		
First Zagreb β index	$M_1^{\beta ve}$	$\sum_{uv\in E} [\aleph_{ve}(u) + \aleph_{ve}(v)]$
Second Zagreb β index	$M_2^{\beta ve}$	$\sum_{uv\in E} [\aleph_{ve}(u) \times \aleph_{ve}(v)]$
Harmonic index	H^{ve}	$\sum_{uv\in E} \frac{2}{\aleph_{ve}(u) + \aleph_{ve}(v)}$
Sum connectivity index	χ^{ve}	$\sum_{uv\in E} [\aleph_{ve}(u) + \aleph_{ve}(v)]^{-1/2}$
Geometric arithmetic index	GA^{ve}	$\sum_{uv\in E} \frac{2\sqrt{\aleph_{ve}(u) \times \aleph_{ve}(v)}}{(\aleph_{ve}(u) + \aleph_{ve}(v))}$
Atom bond connectivity index	ABC^{ve}	$\sum_{uv\in E} \sqrt{\frac{\aleph_{ve}(u) + \aleph_{ve}(v) - 2}{(\aleph_{ve}(u) \times \aleph_{ve}(v))}}$
Randic index	R^{ve}	$\sum_{uv\in E} [\aleph_{ve}(u) \times \aleph_{ve}(v)]^{-1/2}$
First Zagreb α index	$M_1^{\alpha ve}$	$\sum_{v\in V(H)} \aleph_{ve}(v)^2$

$$H(T) = \sum_{uv\in E(T)} \frac{2}{\deg_u + \deg_v}. \tag{6}$$

To read more on harmonic index, see [31, 32]. Zhou and Trinajstic defined the sum-connectivity index (χ) in 2009 [33]. The following formula is used to compute the χ index:

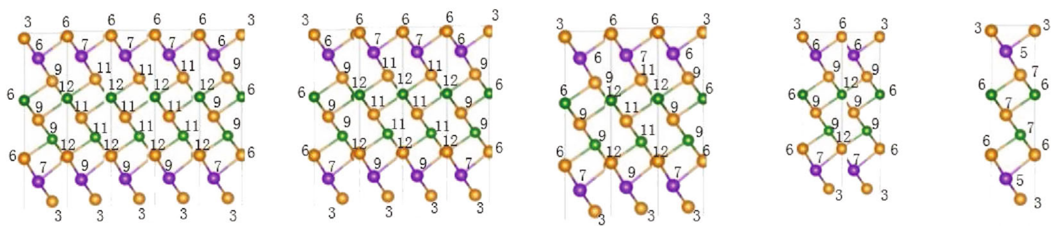
$$\chi(T) = \sum_{uv\in E(T)} \frac{2}{(\deg_u + \deg_v)^{-1/2}}. \tag{7}$$

See [34–43] for further information on these defined topological indices.

Let T be a connected graph and $e = uv \in E(T)$. The ev-degree of the edge e, denoted by $\aleph_{ev}(e)$, is equals the number of vertices in union of the closed neighborhoods of u and v. For any triangle free connected graph T, $\aleph_{ev}(e) = \aleph_{ev}(uv) = \deg(u) + \deg(v)$. The ve-degree of the vertex v, denoted by $\aleph_{ve}(v)$, is equals to the number of different edges that incident to any vertex from the closed neighborhood of v. The mathematical formulas for some of the ev-degree and ve-degree-based indices are presented in Table 1.

2. Ge-Sb-Te Superlattice

Metalloids are normal elements that have properties between metal and nonmetals. Metalloids such as germanium (Ge), antimony (Sb), and tellurium (Te) (GST) with few other elements have been found in the outer layer of the earth crust [44]. They are also formed in an environment by the materials



n = 5 n = 4 n = 3 n = 2 n = 1

Figure 1: Molecular structure of the Ge-Sb-Te superlattice and numbering shows the ve-degrees of vertices.

Table 2: The vertices ve-degrees of Ge-Sb-Te superlattice.

deg (u)	$\aleph_{ve}(u)$	Frequency
1	3	$n+2$
2	6	$n+3$
3	6	2
3	7	n
3	9	$n+4$
3	11	$3n-6$
4	12	$2n-2$

containing both inorganic and organic mixtures in addition to other normal synthetics. These metalloids result in the production of heat, electricity intermediates, and large structured oxides. The free use of such metalloids is restricted because of the potential risks they posed to humans and unpredictability of modern abuse of these elements [45].

Some researchers have focused their attention in modifying these materials into forms that are useful in human life for various fields. For example, the use of the GST alloy in the form of thin films as the two-dimensional (2D) transition metal dichalcogenides has comparable applications in science and technology [46]. Cationic elements, such as group IVA (Sn and Pb), group IIIA (In and Ga), and transition metals are used to construct these GST alloy [47]. The physicochemical properties of Ge-Sb-Te (GST) can be utilized for sensing, as well as in thermoelectric, nonvolatile RAM and face change properties [48, 49]. This can help to improve the bandgap energy of GST. The 2D transition metal dichalcogenides show new properties and are primarily distinct from pure transition bulk compounds [50]. The phase change materials/memory properties of the Ge, Sb, and Te (GST) complex with a group of chalcogenides are a promising technology that have been well known for a considerable amount of time [51, 52]. We denote the structure of Ge-Sb-Te superlattice by SL. The molecular structure of Ge-Sb-Te superlattice is depicted in Figure 1. The structure of SL has $9n+3$ vertices and $13n$ edges. Let V_i denote the vertex set containing the vertices of SL of degree i. Then, the vertex set $V(SL)$ can be partitioned in to four sets with $|V_1| = n+2$, $|V_2| = n+3$, $|V_3| = 5n$, and $|V_4| = 2n-2$. Let $E_{(i,j)}$ denote the edge set containing the edges of SL with end vertices of degree i and degree j, respectively. The edge set of SL can be partitioned based on the degree of end vertices as follows: $|E_{(1,3)}| = n+2$, $|E_{(2,3)}| = 2n+6$, $|E_{(3,3)}| = 2n$, and $|E_{(3,4)}| = 8n-8$. Tables 2 and 3 depict the partition

Table 3: Edge partition of Ge-Sb-Te superlattice.

Edge	$(\aleph_{ve}(u), \aleph_{ve}(v))$	Frequency
E_I°	(3, 6)	2
E_{II}°	(3, 7)	2
E_{III}°	(3, 9)	$n-2$
E_{IV}°	(6, 6)	2
E_V°	(6, 7)	$2n-2$
E_{VI}°	(6, 9)	6
E_{VII}°	(6, 9)	2
E_{VIII}°	(9, 9)	2
E_{IX}°	(7, 11)	$n-2$
E_X°	(11, 11)	$n-2$
E_{XI}°	(7, 12)	2
E_{XII}°	(9, 12)	$2n+2$
E_{XIII}°	(11, 12)	$6n-12$

Table 4: Ev-degrees of edges of Ge-Sb-Te superlattice.

$E_{(\deg(u),\deg(v))}$	$\aleph_{ev}(e)$	Frequency
$E_{(1,3)}$	4	$n+2$
$E_{(2,3)}$	5	$2n+6$
$E_{(3,3)}$	6	$2n$
$E_{(3,4)}$	7	$8n-8$

of SL for $n \geq 2$. In the next theorem, we compute the ev-degree Randic and Zagreb index of SL.

3. Main Results

Theorem 1. *Let $n \geq 1$; then, ev-degree Zagreb and Randic index of Ge-Sb-Te superlattice (SL) are*

$$M^{ev}(SL) = 530n - 210,$$
$$R^{ev}(SL) = \left(\frac{1}{2} + \frac{2}{\sqrt{5}} + \frac{2}{\sqrt{6}} + \frac{8}{\sqrt{7}}\right)n + \frac{6}{\sqrt{5}} - \frac{8}{\sqrt{7}} + 1. \tag{8}$$

Proof. We use Table 4 to compute the ev-degree Randic and Zagreb indices of SL based on the ev-degree of the edges.

$$\begin{aligned}M^{ev}(SL) &= \sum_{e\in E(SL)} \aleph_{ev}(e)^2, = (4)^2\left|E_{(1,3)}\right| + (5)^2\left|E_{(2,3)}\right| \\ &\quad + (6)^2\left|E_{(3,3)}\right| + (7)^2\left|E_{(3,4)}\right| = (4)^2(n+2) \\ &\quad + (5)^2(2n+6) + (6)^2(2n) + (7)^2(8n-8) \\ &= 530n - 210,\end{aligned}$$

$$\begin{aligned}R^{ev}(SL) &= \sum_{e\in E(SL)} \aleph_{ev}(e)^{-1/2}, = (4)^{-1/2}\left|E_{(1,3)}\right| + (5)^{-1/2}\left|E_{(2,3)}\right| \\ &\quad + (6)^{-1/2}\left|E_{(3,3)}\right| + (7)^{-1/2}\left|E_{(3,4)}\right| = (4)^{-1/2}(n+2) \\ &\quad + (5)^{-1/2}(2n+6) + (6)^{-1/2}(2n) + (7)^{-1/2}(8n-8) \\ &= \left(\frac{1}{2} + \frac{2}{\sqrt{5}} + \frac{2}{\sqrt{6}} + \frac{8}{\sqrt{7}}\right)n + \frac{6}{\sqrt{5}} - \frac{8}{\sqrt{7}} + 1.\end{aligned} \tag{9}$$

□

Numerical computation and plots of the results of the ev-degree-based indices show an increasing behavior as we increase the value of n. Topological indices are helpful to predict physical properties. Zhong et al. [14] study the QSPR of phytochemicals that are used for screening against SARS-CoV-23CL^{pro} using ev and ve-degree-based topological descriptors. They analyzed that in ev-degree-based indices, the M^{ev} predict the molecular weight better than R^{ev}. Recently, Rauf et al. [15] developed the relationship and examine that π-electron energy can be predicted by R^{ev} using linear regression model at significant level 99%. As a result, the data presented here will be useful in determining the Ge-Sb-Te superlattice's physical properties.

Theorem 2. *Let SL denote the structure of Ge-Sb-Te superlattice and $n \geq 2$, then*

$$M_1^{\alpha ve}(SL) = 826n - 492. \tag{10}$$

Proof. From the structure of Ge-Sb-Te superlattice (SL), we partitioned the vertex set in to seven partitions. This partition is depicted in Table 2. □

Using Table 2, we calculate the $M_1^{\alpha ve}$ index based on ve-degrees as follows:

$$M_1^{\alpha ve}(SL) = \sum_{v\in V(SL)} \aleph_{ve}(v)^2,$$

$$\begin{aligned}M_1^{\alpha ve}(Sl) &= (3)^2(n+2) + (6)^2(n+3) + (6)^2(2) + (7)^2(n) \\ &\quad + (9)^2(n+4) + (11)^2(3n-6) + (12)^2(2n-2) \\ &= 826n - 492.\end{aligned} \tag{11}$$

Numerical computation and plot of the $M_1^{\alpha ve}$ show an increasing behavior of $M_1^{\alpha ve}$ as we increase the value of n. Ediz [10] examines that the $M_1^{\alpha ve}$ predicts the acentric factor. Zhong et al. developed the relationship between physio-chemical properties (binding affinity, docking score, MW, and TPS) and topological indices (ve- and ev-degree based) [14]. Zhong et al. analyze that the $M_1^{\alpha ve}$ predicts the molecular weight better than R^{ev}. So, the above result of Theorem 2 is helpful to measure the physical property of Ge-Sb-Te superlattice.

Theorem 3. *Let SL denote the structure of Ge-Sb-Te superlattice and $n \geq 2$, then*

$$M_1^{\beta ve}(SL) = 258n - 108,$$

$$M_2^{\beta ve}(SL) = 1317n - 990,$$

$$\begin{aligned}ABC^{ve}(SL) &= \left(\sqrt{\frac{10}{27}} + 2\sqrt{\frac{11}{42}} + \sqrt{\frac{16}{77}} + \sqrt{\frac{20}{121}} + 2\sqrt{\frac{19}{108}} + 6\sqrt{\frac{21}{132}}\right)n + 2\sqrt{\frac{7}{18}} + 2\sqrt{\frac{8}{21}} + \sqrt{\frac{10}{27}} + 2\sqrt{\frac{10}{36}} \\ &\quad - 2\sqrt{\frac{11}{42}} + 6\sqrt{\frac{13}{54}} + 2\sqrt{\frac{13}{54}} + 2\sqrt{\frac{16}{81}} - 2\sqrt{\frac{16}{77}} \\ &\quad - 2\sqrt{\frac{20}{121}} + 2\sqrt{\frac{17}{84}} + 2\sqrt{\frac{19}{108}} - 12,.\end{aligned}$$

$$\begin{aligned}GA^{ve}(SL) &= \left(\frac{\sqrt{27}}{6} + \frac{4\sqrt{42}}{13} + \frac{\sqrt{77}}{9} + \frac{4\sqrt{108}}{21} + \frac{12\sqrt{132}}{23} + 1\right)n + \frac{4\sqrt{18}}{9} + \frac{2\sqrt{21}}{5} - \frac{\sqrt{27}}{3} \\ &\quad - \frac{4\sqrt{42}}{13} + \frac{16\sqrt{54}}{15} - \frac{2\sqrt{77}}{9} + \frac{4\sqrt{84}}{19} + \frac{4\sqrt{108}}{21} \\ &\quad - \frac{24\sqrt{132}}{23} + 3,\end{aligned}$$

$$H^{ve}(SL) = \frac{575453}{414414}n + \frac{15336812}{19684665},$$

$$\begin{aligned}\chi^{ve}(SL) &= \left(\frac{1}{\sqrt{12}} + \frac{2}{\sqrt{13}} + \frac{1}{\sqrt{18}} + \frac{1}{\sqrt{22}} + \frac{2}{\sqrt{21}} + \frac{6}{\sqrt{23}}\right) \\ &\quad \cdot n + \frac{2}{\sqrt{9}} + \frac{2}{\sqrt{10}} - \frac{2}{\sqrt{13}} + \frac{8}{\sqrt{15}} - \frac{2}{\sqrt{22}} \\ &\quad + \frac{2}{\sqrt{19}} + \frac{2}{\sqrt{21}} - \frac{12}{\sqrt{23}},\end{aligned}$$

$$\begin{aligned}R^{ve}(SL) &= \left(\frac{1}{\sqrt{27}} + \frac{2}{\sqrt{42}} + \frac{1}{\sqrt{77}} + \frac{1}{11} + \frac{2}{\sqrt{108}} + \frac{6}{\sqrt{132}}\right) \\ &\quad \cdot n + \frac{2}{\sqrt{18}} + \frac{2}{\sqrt{21}} - \frac{2}{\sqrt{27}} + \frac{1}{3} - \frac{2}{\sqrt{42}} + \frac{8}{\sqrt{54}} \\ &\quad + \frac{2}{9} - \frac{2}{\sqrt{77}} - \frac{2}{11} + \frac{2}{\sqrt{84}} + \frac{2}{\sqrt{108}} - \frac{12}{\sqrt{132}}.\end{aligned} \tag{12}$$

Proof. To compute these indices, we must first determine the edge partition of Ge-Sb-Te superlattice based on the ve-degree of end vertices. This partition is depicted in in Table 3. Figure 1 can be helpful to understand the partition. Using this partition, theses indices can be computed as follows:

$$\begin{aligned}M_1^{\beta ve}(SL) &= \sum_{uv\in E(SL)}(\aleph_{ve}(u)+\aleph_{ve}(v)), = (9)|E_I^\diamond| + (10)|E_{II}^\diamond| \\ &\quad + (12)|E_{III}^\diamond| + (12)|E_{IV}^\diamond| + (13)|E_V^\diamond| + (15)|E_{VI}^\diamond| \\ &\quad + (15)|E_{VII}^\diamond| + (18)|E_{VIII}^\diamond| + (18)|E_{IX}^\diamond| \\ &\quad + (22)|E_X^\diamond| + (19)|E_{XI}^\diamond| + (21)|E_{XII}^\diamond| + (23)|E_{XIII}^\diamond| \\ &= (9)(2) + (10)(2) + (12)(n-2) + (12)(2) \\ &\quad + (13)(2n-2) + (15)(6) + (15)(2) + (18)(2) \\ &\quad + (18)(n-2) + (22)(n-2) + (19)(2) \\ &\quad + (21)(2n+2) + (23)(6n-12) = 258n - 108,\end{aligned}$$

$$\begin{aligned}M_2^{\beta ve}(SL) &= \sum_{uv\in E(SL)}(\aleph_{ve}(u)\times\aleph_{ve}(v)), = (18)|E_I^\diamond| + (21)|E_{II}^\diamond| \\ &\quad + (27)|E_{III}^\diamond| + (36)|E_{IV}^\diamond| + (42)|E_V^\diamond| + (54)|E_{VI}^\diamond| \\ &\quad + (54)|E_{VII}^\diamond| + (81)|E_{VIII}^\diamond| + (77)|E_{IX}^\diamond| + (121) \\ &\quad \cdot |E_X^\diamond| + (84)|E_{XI}^\diamond| + (108)|E_{XII}^\diamond| + (132)|E_{XIII}^\diamond| \\ &= (18)(2) + (21)(2) + (27)(n-2) + (36)(2) \\ &\quad + (42)(2n-2) + (54)(6) + (54)(2) + (81)(2) \\ &\quad + (77)(n-2) + (121)(n-2) + (84)(2) \\ &\quad + (108)(2n+2) + (132)(6n-12) = 1317n - 990,\end{aligned}$$

$$\begin{aligned}ABC^{ve}(SL) &= \sum_{uv\in E(SL)}\sqrt{\frac{\aleph_{ve}(u)+\aleph_{ve}(v)-2}{(\aleph_{ve}(u)\times\aleph_{ve}(v))}}, = \left(\sqrt{\frac{7}{18}}\right)|E_I^\diamond| \\ &\quad + \left(\sqrt{\frac{8}{21}}\right)|E_{II}^\diamond| + \left(\sqrt{\frac{10}{27}}\right)|E_{III}^\diamond| + \left(\sqrt{\frac{10}{36}}\right) \\ &\quad \cdot |E_{IV}^\diamond| + \left(\sqrt{\frac{11}{42}}\right)|E_V^\diamond| ++ \left(\sqrt{\frac{13}{54}}\right)|E_{VI}^\diamond| \\ &\quad + \left(\sqrt{\frac{13}{54}}\right)|E_{VII}^\diamond| + \left(\sqrt{\frac{16}{81}}\right)|E_{VIII}^\diamond| + \left(\sqrt{\frac{16}{77}}\right) \\ &\quad \cdot |E_{IX}^\diamond| + \left(\sqrt{\frac{20}{121}}\right)|E_X^\diamond| + \left(\sqrt{\frac{17}{84}}\right)|E_{XI}^\diamond| \\ &\quad + \left(\sqrt{\frac{19}{108}}\right)|E_{XII}^\diamond| + \left(\sqrt{\frac{21}{132}}\right)|E_{XIII}^\diamond| \\ &= \left(\sqrt{\frac{7}{18}}\right)(2) + \left(\sqrt{\frac{8}{21}}\right)(2) + \left(\sqrt{\frac{10}{27}}\right)(n-2) \\ &\quad + \left(\sqrt{\frac{10}{36}}\right)(2) + \left(\sqrt{\frac{11}{42}}\right)(2n-2) \\ &\quad + \left(\sqrt{\frac{13}{54}}\right)(6) + \left(\sqrt{\frac{13}{54}}\right)(2) + \left(\sqrt{\frac{16}{81}}\right)(2) \\ &\quad + \left(\sqrt{\frac{16}{77}}\right)(n-2) + \left(\sqrt{\frac{20}{121}}\right)(n-2) \\ &\quad + \left(\sqrt{\frac{17}{84}}\right)(2) + \left(\sqrt{\frac{19}{108}}\right)(2n+2) + \left(\sqrt{\frac{21}{132}}\right) \\ &\quad \cdot (6n-12) = \left(\sqrt{\frac{10}{27}} + 2\sqrt{\frac{11}{42}} + \sqrt{\frac{16}{77}} + \sqrt{\frac{20}{121}}\right. \\ &\quad \left. + 2\sqrt{\frac{19}{108}} + 6\sqrt{\frac{21}{132}}\right)n + 2\sqrt{\frac{7}{18}} + 2\sqrt{\frac{8}{21}} \\ &\quad - 2\sqrt{\frac{10}{27}} + 2\sqrt{\frac{10}{36}} - 2\sqrt{\frac{11}{42}} + 6\sqrt{\frac{13}{54}} + 2\sqrt{\frac{13}{54}} \\ &\quad + 2\sqrt{\frac{16}{81}} - 2\sqrt{\frac{16}{77}} - 2\sqrt{\frac{20}{121}} + 2\sqrt{\frac{17}{84}} \\ &\quad + 2\sqrt{\frac{19}{108}} - 12\sqrt{\frac{21}{132}},\end{aligned}$$

$$\begin{aligned}GA^{ve}(SL) &= \sum_{uv\in E(SL)}\frac{2\sqrt{\aleph_{ve}(u)\times\aleph_{ve}(v)}}{(\aleph_{ve}(u)+\aleph_{ve}(v))}, = \left(\frac{2\sqrt{18}}{9}\right)|E_I^\diamond| \\ &\quad + \left(\frac{2\sqrt{21}}{10}\right)|E_{II}^\diamond| + \left(\frac{2\sqrt{27}}{12}\right)|E_{III}^\diamond| + \left(\frac{2\sqrt{36}}{12}\right) \\ &\quad \cdot |E_{IV}^\diamond| + \left(\frac{2\sqrt{42}}{13}\right)|E_V^\diamond| + \left(\frac{2\sqrt{54}}{15}\right)|E_{VI}^\diamond| \\ &\quad + \left(\frac{2\sqrt{54}}{15}\right)|E_{VII}^\diamond| + \left(\frac{2\sqrt{81}}{18}\right)|E_{VIII}^\diamond| \\ &\quad + \left(\frac{2\sqrt{77}}{18}\right)|E_{IX}^\diamond| + \left(\frac{2\sqrt{121}}{22}\right)|E_X^\diamond| + \left(\frac{2\sqrt{84}}{19}\right) \\ &\quad \cdot |E_{XI}^\diamond| + \left(\frac{2\sqrt{108}}{21}\right)|E_{XII}^\diamond| + \left(\frac{2\sqrt{132}}{23}\right)|E_{XIII}^\diamond| \\ &= \left(\frac{2\sqrt{18}}{9}\right)(2) + \left(\frac{2\sqrt{21}}{10}\right)(2) + \left(\frac{2\sqrt{27}}{12}\right)(n-2) \\ &\quad + \left(\frac{2\sqrt{36}}{12}\right)(2) + \left(\frac{2\sqrt{42}}{13}\right)(2n-2) + \left(\frac{2\sqrt{54}}{15}\right) \\ &\quad \cdot (6) + \left(\frac{2\sqrt{54}}{15}\right)(2) + \left(\frac{2\sqrt{81}}{18}\right)(2) + \left(\frac{2\sqrt{77}}{18}\right) \\ &\quad \cdot (n-2) + \left(\frac{2\sqrt{121}}{22}\right)(n-2) + \left(\frac{2\sqrt{84}}{19}\right)(2) \\ &\quad + \left(\frac{2\sqrt{108}}{21}\right)(2n+2) + \left(\frac{2\sqrt{132}}{23}\right)(6n-12) \\ &= \left(\frac{\sqrt{27}}{6} + \frac{4\sqrt{42}}{13} + \frac{\sqrt{77}}{9} + \frac{4\sqrt{108}}{21} + \frac{12\sqrt{132}}{23} + 1\right)\end{aligned}$$

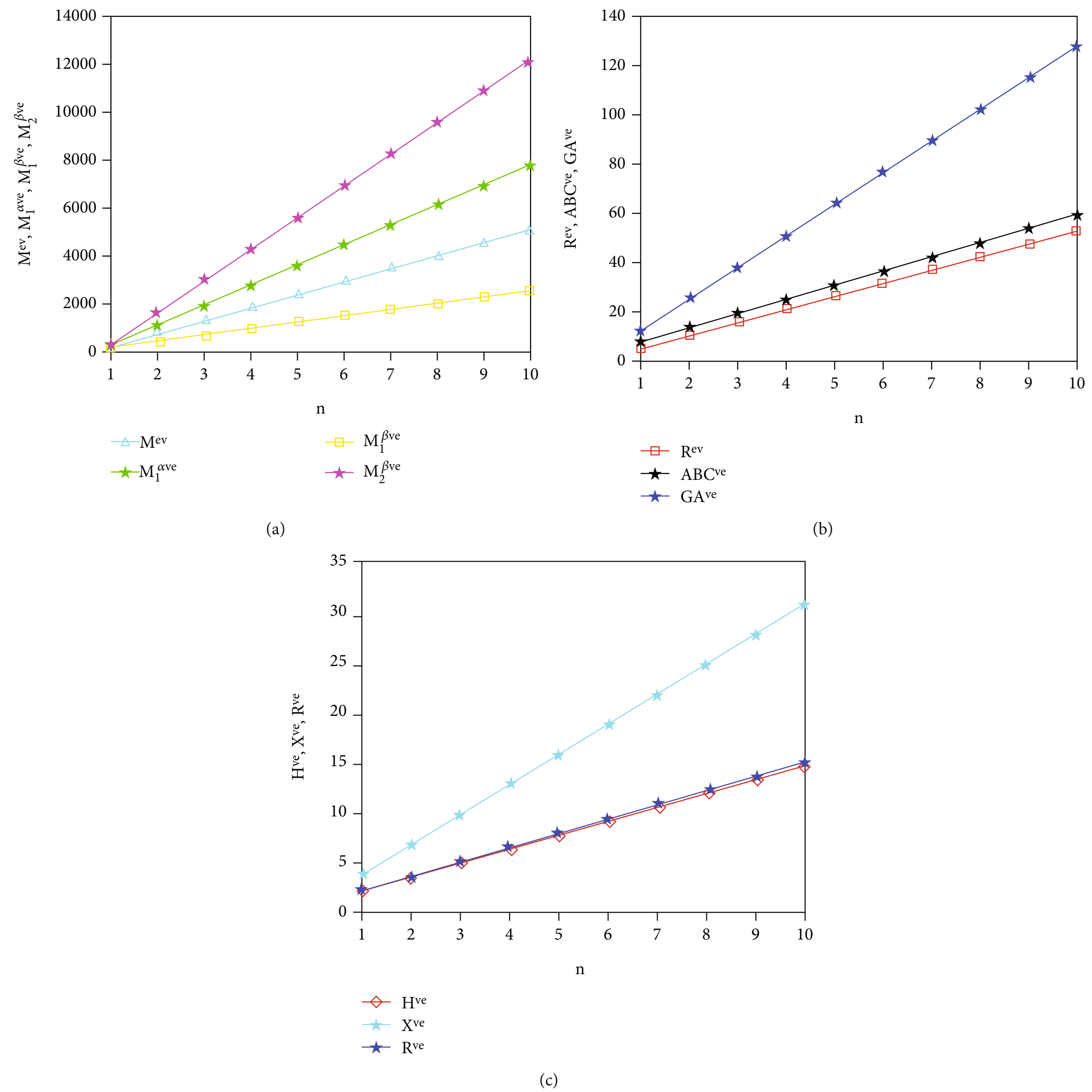


Figure 2: Visual behavior of (a) ev-degree Zagreb index (M^{ev}), ve-degree first Zagreb α index ($M_1^{\alpha ve}$), first Zagreb β index ($M_1^{\beta ve}$), and second Zagreb β index ($M_2^{\beta ve}$); (b) ev-degree Randic index (R^{ev}), atom bond connectivity (ABC^{ve}), and geometric arithmetic (R^{ve}) index; and (c) ve-degree Randic (R^{ve}), Harmonic (H^{ve}), and sum connectivity (χ^{ve}) index.

$$
n + \frac{4\sqrt{18}}{9} + \frac{2\sqrt{21}}{5} - \frac{\sqrt{27}}{3} - \frac{4\sqrt{42}}{13} + \frac{16\sqrt{54}}{15} - \frac{2\sqrt{77}}{9} + \frac{4\sqrt{84}}{19} + \frac{4\sqrt{108}}{21} - \frac{24\sqrt{132}}{23} + 3,
$$

$$
\begin{aligned}
H^{ve}(SL) = \sum_{uv\in E(SL)} \frac{2}{\aleph_{ve}(u) + \aleph_{ve}(v)}, &= \left(\frac{2}{9}\right)|E_I^{\diamond}| + \left(\frac{2}{10}\right)|E_{II}^{\diamond}| \\
&+ \left(\frac{2}{12}\right)|E_{III}^{\diamond}| + \left(\frac{2}{12}\right)|E_{IV}^{\diamond}| + \left(\frac{2}{13}\right)|E_V^{\diamond}| + \left(\frac{2}{15}\right) \\
&\cdot |E_{VI}^{\diamond}| + \left(\frac{2}{15}\right)|E_{VII}^{\diamond}| + \left(\frac{2}{18}\right)|E_{VIII}^{\diamond}| + \left(\frac{2}{18}\right)|E_{IX}^{\diamond}| \\
&+ \left(\frac{2}{22}\right)|E_X^{\diamond}| + \left(\frac{2}{19}\right)|E_{XI}^{\diamond}| + \left(\frac{2}{21}\right)|E_{XII}^{\diamond}| + \left(\frac{2}{23}\right) \\
&\cdot |E_{XIII}^{\diamond}| = \left(\frac{2}{9}\right)(2) + \left(\frac{2}{10}\right)(2) + \left(\frac{2}{12}\right)(n-2) \\
&+ \left(\frac{2}{12}\right)(2) + \left(\frac{2}{13}\right)(2n-2) + \left(\frac{2}{15}\right)(6) + \left(\frac{2}{15}\right)
\end{aligned}
$$

$$(2) + \left(\frac{2}{18}\right)(2) + \left(\frac{2}{18}\right)(n-2) + \left(\frac{2}{22}\right)(n-2) + \left(\frac{2}{19}\right)(2) + \left(\frac{2}{21}\right)(2n+2) + \left(\frac{2}{23}\right)(6n-12) = \frac{575453}{414414}n + \frac{15336812}{19684665},$$

$$\chi^{ve}(SL) = \sum_{uv\in E(SL)} (\aleph_{ve}(u) + \aleph_{ve}(v))^{-1/2}, = \left(\frac{1}{\sqrt{9}}\right)|E_I^{\diamond}| + \left(\frac{1}{\sqrt{10}}\right)|E_{II}^{\diamond}| + \left(\frac{1}{\sqrt{12}}\right)|E_{III}^{\diamond}| + \left(\frac{1}{\sqrt{12}}\right)|E_{IV}^{\diamond}| + \left(\frac{1}{\sqrt{13}}\right)|E_V^{\diamond}| + \left(\frac{1}{\sqrt{15}}\right)|E_{VI}^{\diamond}| + \left(\frac{1}{\sqrt{15}}\right)|E_{VII}^{\diamond}| + \left(\frac{1}{\sqrt{18}}\right)|E_{VIII}^{\diamond}| + \left(\frac{1}{\sqrt{18}}\right)|E_{IX}^{\diamond}| + \left(\frac{1}{\sqrt{22}}\right)|E_X^{\diamond}| + \left(\frac{1}{\sqrt{19}}\right)|E_{XI}^{\diamond}| + \left(\frac{1}{\sqrt{21}}\right)|E_{XII}^{\diamond}| + \left(\frac{1}{\sqrt{23}}\right)|E_{XIII}^{\diamond}|$$
$$= \left(\frac{1}{\sqrt{9}}\right)(2) + \left(\frac{1}{\sqrt{10}}\right)(2) + \left(\frac{1}{\sqrt{12}}\right)(n-2) + \left(\frac{1}{\sqrt{12}}\right)(2) + \left(\frac{1}{\sqrt{13}}\right)(2n-2) + \left(\frac{1}{\sqrt{15}}\right)(6) + \left(\frac{1}{\sqrt{15}}\right)(2) + \left(\frac{1}{\sqrt{18}}\right)(2) + \left(\frac{1}{\sqrt{18}}\right)(n-2) + \left(\frac{1}{\sqrt{22}}\right)(n-2) + \left(\frac{1}{\sqrt{19}}\right)(2) + \left(\frac{1}{\sqrt{21}}\right)(2n+2) + \left(\frac{1}{\sqrt{23}}\right)(6n-12) = \left(\frac{1}{\sqrt{12}} + \frac{2}{\sqrt{13}} + \frac{1}{\sqrt{18}} + \frac{1}{\sqrt{22}} + \frac{2}{\sqrt{21}} + \frac{6}{\sqrt{23}}\right)n + \frac{2}{\sqrt{9}} + \frac{2}{\sqrt{10}} - \frac{2}{\sqrt{13}} + \frac{8}{\sqrt{15}} - \frac{2}{\sqrt{22}} + \frac{2}{\sqrt{19}} + \frac{2}{\sqrt{21}} - \frac{12}{\sqrt{23}},$$

$$\mathrm{R}^{ve}(SL) = \sum_{uv\in E(SL)} (\aleph_{ve}(u) \times \aleph_{ve}(v))^{-1/2}, = (18)^{-1/2}|E_I^{\diamond}| + (21)^{-1/2}|E_{II}^{\diamond}| + (27)^{-1/2}|E_{III}^{\diamond}| + (36)^{-1/2}|E_{IV}^{\diamond}| + (42)^{-1/2}|E_V^{\diamond}| + (54)^{-1/2}|E_{VI}^{\diamond}| + (54)^{-1/2}|E_{VII}^{\diamond}| + (81)^{-1/2}|E_{VIII}^{\diamond}| + (77)^{-1/2}|E_{IX}^{\diamond}| + (121)^{-1/2}|E_X^{\diamond}| + (84)^{-1/2}|E_{XI}^{\diamond}| + (108)^{-1/2}|E_{XII}^{\diamond}| + (132)^{-1/2}|E_{XIII}^{\diamond}|$$
$$= \left(\frac{1}{\sqrt{18}}\right)(2) + \left(\frac{1}{\sqrt{21}}\right)(2) + \left(\frac{1}{\sqrt{27}}\right)(n-2) + \left(\frac{1}{\sqrt{36}}\right)(2) + \left(\frac{1}{\sqrt{42}}\right)(2n-2) + \left(\frac{1}{\sqrt{54}}\right)(6) + \left(\frac{1}{\sqrt{54}}\right)(2) + \left(\frac{1}{\sqrt{81}}\right)(2) + \left(\frac{1}{\sqrt{77}}\right)(n-2) + \left(\frac{1}{\sqrt{121}}\right)(n-2) + \left(\frac{1}{\sqrt{84}}\right)(2) + \left(\frac{1}{\sqrt{108}}\right) \cdot (2n+2) + \left(\frac{1}{\sqrt{132}}\right)(6n-12)$$
$$= \left(\frac{1}{\sqrt{27}} + \frac{2}{\sqrt{42}} + \frac{1}{\sqrt{77}} + \frac{1}{11} + \frac{2}{\sqrt{108}} + \frac{6}{\sqrt{132}}\right)n + \frac{2}{\sqrt{18}} + \frac{2}{\sqrt{21}} - \frac{2}{\sqrt{27}} + \frac{1}{3} - \frac{2}{\sqrt{42}} + \frac{8}{\sqrt{54}} + \frac{2}{9} - \frac{2}{\sqrt{77}} - \frac{2}{11} + \frac{2}{\sqrt{84}} + \frac{2}{\sqrt{108}} - \frac{12}{\sqrt{132}}. \tag{13}$$

□

Table 5: Numerical computation of indices for Ge-Sb-Te superlattice.

$[n]$	$\mathrm{M}^{ev}(SL)$	$\mathrm{R}^{ev}(SL)$	$\mathrm{M}_1^{\alpha ve}(SL)$	$\mathrm{M}_1^{\beta ve}(SL)$	$\mathrm{M}_2^{\beta ve}(SL)$
[1]	320	5.8942	334	150	327
[2]	850	11.1288	1160	408	1644
[3]	1380	16.3635	1986	666	2961
[4]	1910	21.5981	2812	924	4278
[5]	2440	26.8328	3638	1182	5595
[6]	2970	32.0674	4464	1440	6912
[7]	3500	37.302	5290	1698	8229
[8]	4030	42.5367	6116	1956	9546
[9]	4560	47.7713	6942	2214	10863
[10]	5090	53.006	7768	2472	12180

Table 6: Numerical computation of indices for Ge-Sb-Te superlattice.

$[n]$	$\mathrm{ABC}^{ve}(SL)$	$\mathrm{GA}^{ve}(SL)$	$\mathrm{H}^{ve}(SL)$	$\chi^{ve}(SL)$	$\mathrm{R}^{ve}(SL)$
[1]	7.06318	12.6101	2.1677	3.7565	2.2356
[2]	12.7897	25.4191	3.5563	6.7363	3.6562
[3]	18.5163	38.2280	4.9449	9.7161	5.0768
[4]	24.2428	51.0369	6.3335	12.6959	6.4975
[5]	29.9694	63.8458	7.7221	15.6757	7.9181
[6]	35.6960	76.6547	9.1107	18.6555	9.3387
[7]	41.4225	89.4636	10.4993	21.6353	10.7593
[8]	47.1491	102.273	11.8879	24.6151	12.1799
[9]	52.8756	115.081	13.2765	27.5949	13.6005
[10]	58.6022	127.890	14.6651	30.5747	15.0211

Numerical computation and plots of the results show that the value of these indices increase with the increase in the value of n. Ediz [10] examines that entropy and enthalpy of vaporization can be predicted by ${M_2}^{\beta ve}$ and R^{ve}, respectively. Zhong et al. [14] investigated that the $M_1^{\beta ve}$ predicts the topological polar surface and molecular weight better than other indices. Recently, Rauf et al. examined the relationship and analyzed that the boiling point can be predicted by ABC^{ve}, enthalpy by R^{ve}, and molecular weight by χ^{ve} using linear regression model at significant level 99% [15]. As a result, the results of Theorem 3 can be used to measure Ge-Sb-Te superlattice's physical properties.

Figure 2 depicts a visual representation of all computed data.

4. Numerical Results

It can be seen from Tables 5 and 6 and Figure 2 of indices that an increase in the value of n increases the values of descriptors for Ge-Sb-Te superlattice.

5. Conclusion

Topological indices are essential instruments for approximating and predicting chemical compound characteristics in QSPRs and QSARs. The TI reflects a molecule's biological, physical, and chemical characteristics including flickering point, docking score, melting point, binding affinity, topological polar surface, and forming heat. The ev and ve-degree-based topological descriptors for the molecular structure of Ge-Sb-Te superlattice were calculated in this study to better understand pharmaceutical, chemical, and biological characteristics.

Data Availability

No data is required for this study.

Conflicts of Interest

The authors declare that the publishing of this paper is free of conflicts of interest.

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