




## Characterizing superlattice topologies via fifth $M$ -Zagreb polynomials and structural indices

Hani Shaker<sup>1,a</sup> , Sabeen Javaid<sup>2,b</sup>, Usman Babar<sup>2,c</sup>, Muhammad Kamran Siddiqui<sup>1,d</sup>, Asim Naseem<sup>2,e</sup>

<sup>1</sup> Department of Mathematics, COMSATS University Islamabad, Lahore Campus, Lahore, Pakistan

<sup>2</sup> Department of Mathematics, Government College University, Lahore, Pakistan

Received: 23 September 2023 / Accepted: 30 October 2023

© The Author(s), under exclusive licence to Società Italiana di Fisica and Springer-Verlag GmbH Germany, part of Springer Nature 2023

**Abstract** Graph theory provides a strong framework for evaluating and comprehending atom and molecule connections and interactions. Chemical compounds are represented as graphs with edges and vertices. Topological indices have a wide range of applications in the world of research. Topological indices are used for the prediction of chemical compound's properties (boiling point, strain energy, distortion, and stability). The calculation of various indices and polynomials for a molecular graph of a super lattice demonstrates the utilization of graph theory. In the characterization and analysis of molecular structures, including based on degrees, fifth  $M$ -Zagreb indices, fifth hyper- $M$ -Zagreb indices, fifth  $M_2$ -Zagreb polynomials, fifth  $M_1$ -Zagreb polynomials, and fifth  $M_1$ -Zagreb polynomials in general.

### 1 Introduction

Currently, graph theory seeks to advance and apply several contemporary scientific hypotheses in various branches of chemistry. Typically, nodes and edges make up a graph [8]. A graph consists of vertices (also known as nodes) and edges, which are the lines or arcs that connect any two or more vertices.  $T$  can be used to mathematically depict a graph. Assuming that the basic connected graph  $T=(V, E)$  is given,  $V$  shows nodes or points in the graph. Each vertex is typically labeled with a unique identifier or value, and  $E$  shows the connections or relationships between vertices in the graph. An edge connects two vertices and can be either directed (with a specific direction) or undirected (without any direction). The quantity of elements in  $V$  and the quantity of elements in  $E$ , respectively, determine the order and size of  $T$  [9]. The graph is finished, if all distinct pairs of vertices in  $T$  are in close proximity. There are no isolated vertices, loops, or multiple edges in any of the finite, undirected graphs that are being considered. The vertex degree in a graph ( $T$ ) refers to the count of directly connected vertices to a specific vertex or  $V(T)$ . Polynomials, matrices, and integers can all be used to represent a graph.

Zhang et. al [10] computed the topological indices of generalized molecular graphs and products of chemical graphs. Shao et.al [11] computed Zagreb indices for nanotubes. Gao et.al [12] provided the characterization of carbon graphite. Zhang et. al [13, 14] discussed the physical analysis of heat for the formation and entropy of ceria oxide. Zhang et. al [15, 16] provides an analysis of different molecular structures using topological indices. Liu et.al [27] discuss the smart grid graphs for topological analysis. Lu et.al [28] provided the details about bipolar cubic fuzzy graphs and its chemical applications. Ma et.al [29] provided the classification of integrating knowledge graphs with topological indices. Wu et.al [34] analyzed the application of graph theory teaching method in ideological and political education.

Topological indices are used in chemical graph theory to analyze the molecular topological qualities of molecules. The computation of topological indices in the domain of chemical research enables the examination of the molecular structure's impact on the associated chemical, pharmacological, and biological characteristics of pharmaceutical. By analyzing topological indices, researchers can gain insights into the relationships between molecular topology and various properties and behaviors of pharmaceutical compounds [25]. The QSAR/QSPR research involved the integration of physiochemical characteristics and topological indices, such as the hyper-Zagreb index (which is calculated by summing the square of the vertex degree within the graph), the first multiple Zagreb index

<sup>a</sup> e-mail: hani.uet@gmail.com

<sup>b</sup> e-mail: sabeenjavid99@gmail.com

<sup>c</sup> e-mail: usmanbabar762@yahoo.com

<sup>d</sup> e-mail: kamransiddiqui75@gmail.com (corresponding author)

<sup>e</sup> e-mail: dr.asimnaseem@gcu.edu.pk

(the molecular graph's vertex pairs are multiplied together, and their degrees are summed to compute it), and the second multiple Zagreb index (which is computed by summing the squares of the multiplication of the degrees of each pair of adjacent vertices in the graph results in the product of their degrees). These indices were utilized to analyze the molecular structures of the compounds being studied [26].

## 2 Motivation and interest of researchers

Topological indices are numerical descriptors that offer information about a molecule's structure and behavior. Topological indices based on sums of vertex degrees in a molecular network, in particular, are determined. Here are some reasons why you should use sum degree-based topological indices:

1. Molecular structure–property relationships: Topological indices, which predict the characteristics and activities of molecules based on their structure, have been widely employed in chemoinformatics and drug development. Sum degree-based topological indices can give insights into molecular attributes such as boiling point, solubility, and biological activity by assessing the connectivity and degree distribution of atoms in a molecule.

2. Prediction of stereoselectivity and reactivity: The spatial arrangement of atoms in a molecule, particularly in chiral compounds, is critical in determining biological activity and reactivity. Topological indices based on sum degrees can capture a molecule's symmetry and spatial information, making them valuable for forecasting reaction stereoselectivity.

This article discusses some established and recently developed degree-based topological indices [4, 17]. The graph invariants now known as Zagreb indices were the first vertex-degree-based structure identifiers [18, 19]. A chemical structure called a graph, denoted as  $T$ , is made up of a collection of vertices ( $V$ ) and a set of edges ( $E$ ). The set of vertices includes all the nodes or points in the graph, and the set of edges includes all the connections or links between the vertices. The quantity of edges at a vertex determines its degree of incidence on it (denoted by  $\text{deg}_v$ ). The collection of all vertices that are adjacent to  $v$  is known as the open neighborhood  $N(v)$  vertex constructed the degree-based indices [2, 22]. The degree sum of a vertex's neighbors is represented by the symbol  $S_T(v)$ , this is the total of all degrees of a vertex's neighbors[30].

## 3 Some features of superlattice structures

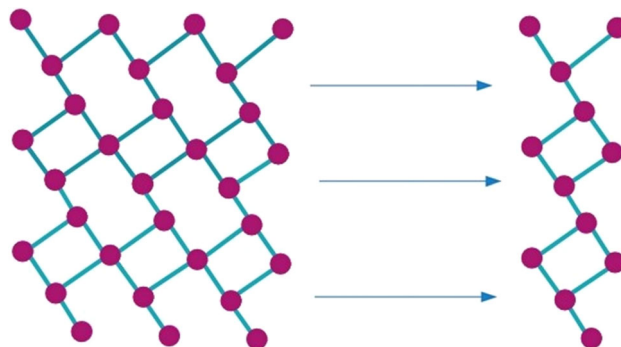
In solid-state physics and materials science, a superlattice is a specialized structure composed of alternating layers of two or more different materials having distinct characteristics and crystal structures. Typically, these layered structures are created utilizing sophisticated growth methods such as molecular beam epitaxy or chemical vapor deposition.

Superlattices have unique and controllable features not seen in the basic materials. Researchers can create and regulate a wide range of physical phenomena by altering the thickness, content, and arrangement of the layers, making these structures very appealing for a variety of technological applications. The confinement and interaction of charge carriers, photons, or phonons inside the layered structure is the basic concept of a superlattice. This confinement causes quantum confinement effects, in which the characteristics of particles are altered as a result of their confinement at nanoscale dimensions.

Superlattices have found use in a variety of sectors, including electronics, optoelectronics, thermoelectrics, quantum computers, and photovoltaics. They have been utilized to improve electronic devices. For more details see Fig. 1.

Vertex sum degrees that are close to a vertex  $u$  is known as  $S_T(u)$  according to Graovac et al [21]. In other words, the sum of all the degrees of the vertices in the graph  $T$  that are directly related to vertex  $u$  is known as  $S_T(u)$ . Inspired by the Graovac indices, V. R. Kulli [23, 24] introduced the general fifth  $M$ -Zagreb indices. For a molecular graph, these indices were created as polynomials. In QSAR/QSPR research, the fifth  $M$ -Zagreb indices, a particular kind of topological index, are frequently employed to examine the molecular structure of a chemical. These indices have shown their capacity to predict a number of physicochemical

**Fig. 1** Superlattice structure



properties of molecules, including surface area, boiling points, and melting points. They are created by computing the total of all of the chemical network’s vertices’ degrees [1], The fifth  $M$ -Zagreb index ( $MZ_5$ ) is a graph-theoretic topological index that describes the degree of branching of a molecule. It is a modification of the original Zagreb index, which sums the degrees of all vertices in a molecule. Quantitative structure–property relationship (QSPR) models have also been created using it to predict a number of molecular physical and chemical properties [5]. The following is a description of these indices.

$$M_1G_5(T) = \sum_{uv \in E(T)} (\xi_T(u) + \xi_T(v)), \tag{1}$$

$$M_2G_5(T) = \sum_{uv \in E(T)} (\xi_T(u)\xi_T(v)). \tag{2}$$

V. R. Kulli created the general fifth  $M$ -Zagreb indices and fifth hyper- $M$ -Zagreb indices in reference to the aforementioned indices. Here is a description of them:

$$M_1^aG_5(T) = \sum_{uv \in E(T)} (\xi_T(u) + \xi_T(v))^a, \tag{3}$$

$$M_2^aG_5(T) = \sum_{uv \in E(T)} (\xi_T(u)\xi_T(v))^a, \tag{4}$$

$$HM_1G_5(T) = \sum_{uv \in E(T)} (\xi_T(u) + \xi_T(v))^2, \tag{5}$$

$$HM_2G_5(T) = \sum_{uv \in E(T)} (\xi_T(u)\xi_T(v))^2. \tag{6}$$

Furthermore, they introduced a revised version of the Zagreb index, that is alternatively referred to as the third Zagreb index or the fifth  $M_3$ -Zagreb index,

$$M_3G_5(T) = \sum_{uv \in E(T)} |\xi_T(u) - \xi_T(v)|. \tag{7}$$

Corresponding the above indices, they defined the General fifth  $M_1$ -Zagreb polynomial and the general fifth  $M_2$ -Zagreb polynomial of a molecular graph  $T$ .

$$M_1^aT_5(T, z) = \sum_{uv \in E(T)} z^{(\xi_T(u)+\xi_T(v))^a}, \tag{8}$$

$$M_2^aG_5(T, z) = \sum_{uv \in E(T)} z^{(\xi_T(u)\xi_T(v))^a}. \tag{9}$$

The fifth  $M_1$ -Zagreb polynomial and the fifth  $M_2$ -Zagreb polynomial of a graph  $T$  are defined

$$M_1G_5(T, z) = \sum_{uv \in E(T)} z^{(\xi_T(u)+\xi_T(v))}, \tag{10}$$

$$M_2G_5(T, z) = \sum_{uv \in E(T)} z^{(\xi_T(u)\xi_T(v))}. \tag{11}$$

The fifth hyper- $M_1$ -Zagreb polynomial and the fifth hyper- $M_2$ -Zagreb polynomial of a graph  $T$  are defined

$$M_1G_5(T, z) = \sum_{uv \in E(T)} z^{(\xi_T(u)+\xi_T(v))^2}, \tag{12}$$

$$M_2G_5(T, z) = \sum_{uv \in E(T)} z^{(\xi_T(u)\xi_T(v))^2}. \tag{13}$$

References provide additional resources and literature pertaining to the study of topological indices [3, 6, 7, 20, 32].

In Fig. 2, we have presented the bibliometric analysis of the fifth Zagreb  $M$ -polynomial keywords in different manners. In this analysis, it can be seen easily that fifth Zagreb  $M$ -polynomial keywords are mostly discuss in different forms.

In Fig. 3, we have presented the bibliometric analysis of the fifth Zagreb  $M$ -polynomial by different authors in world.

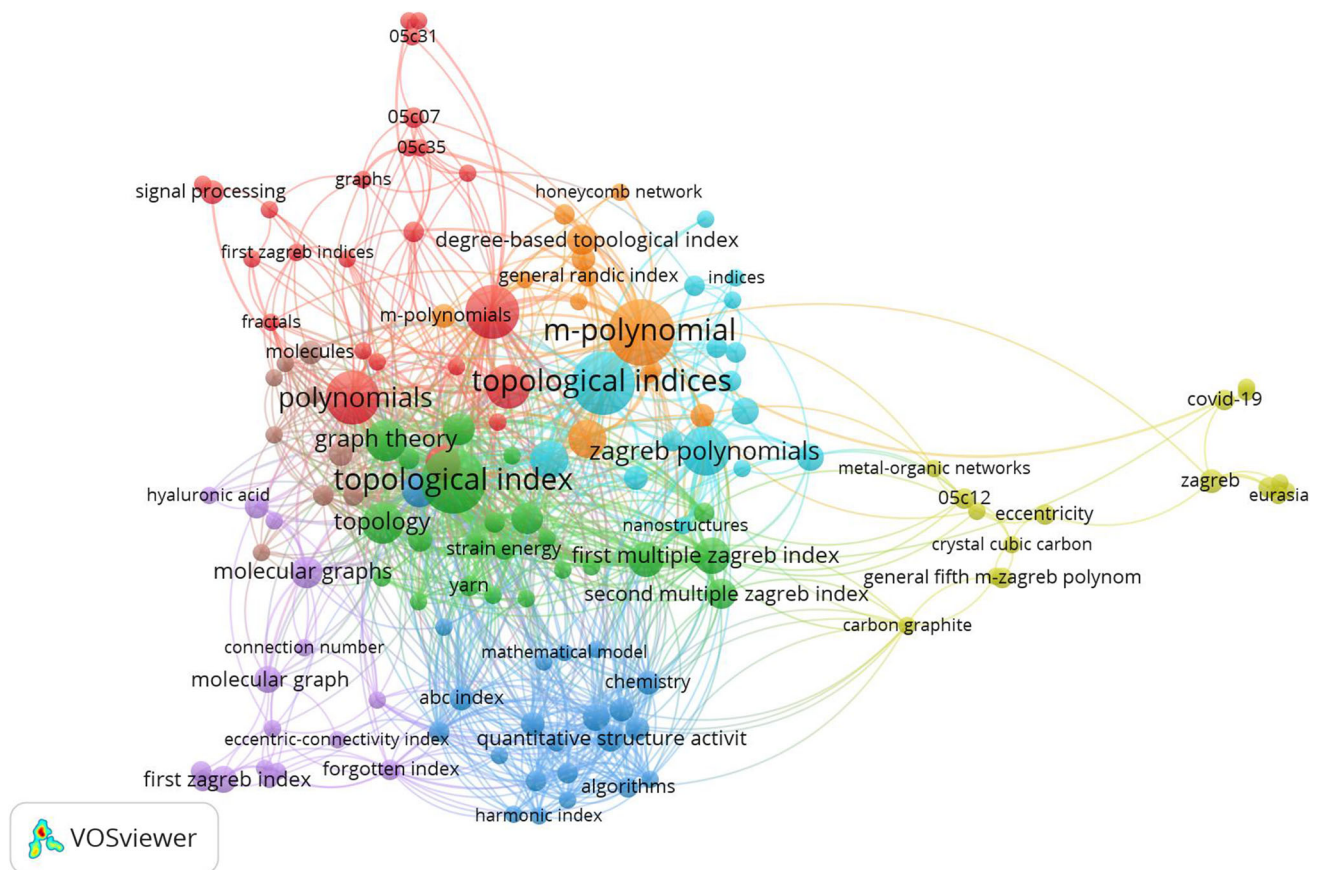


Fig. 2 Bibliometric value of fifth Zagreb  $M$ -polynomial with respect to other topological indices

4 Main results

An arrangement of alternating layers of several materials is known as a superlattice. Phase-change memory technology employs a material known as Ge-Sb-Te superlattice. It consists of alternating layers of germanium (Ge), antimony (Sb), and tellurium (Te) atoms [31]. The usual superlattice is quite tiny, and these layers are commonly measured in nanometers. These structures are utilized in the development of novel semiconductor forms that display characteristics distinct from those of the constituent materials. The arrangement of atoms within the Ge-Sb-Te superlattice at the molecular level can be described as a series of crystalline layers, with each layer composed of a repeating pattern of atoms[33]. The layers are arranged in a way that creates a specific atomic arrangement that allows for rapid changes in electrical conductivity. Superlattice’s composition have  $9n + 3$  vertices and  $13n$  edges see Table 1.

**Theorem 4.1** Consider the superlattice structure,  $M_1G_5(T)$  of fifth  $M$ -Zagreb index given a molecular graph, that is equivalent to:

$$M_1G_5(T) = 258n - 108.$$

*Proof* Let  $T$  be the superlattice structure. From Eq. (1),

$$M_1G_5(T) = \sum_{uv \in E(T)} (\$T(u) + \$T(v)).$$

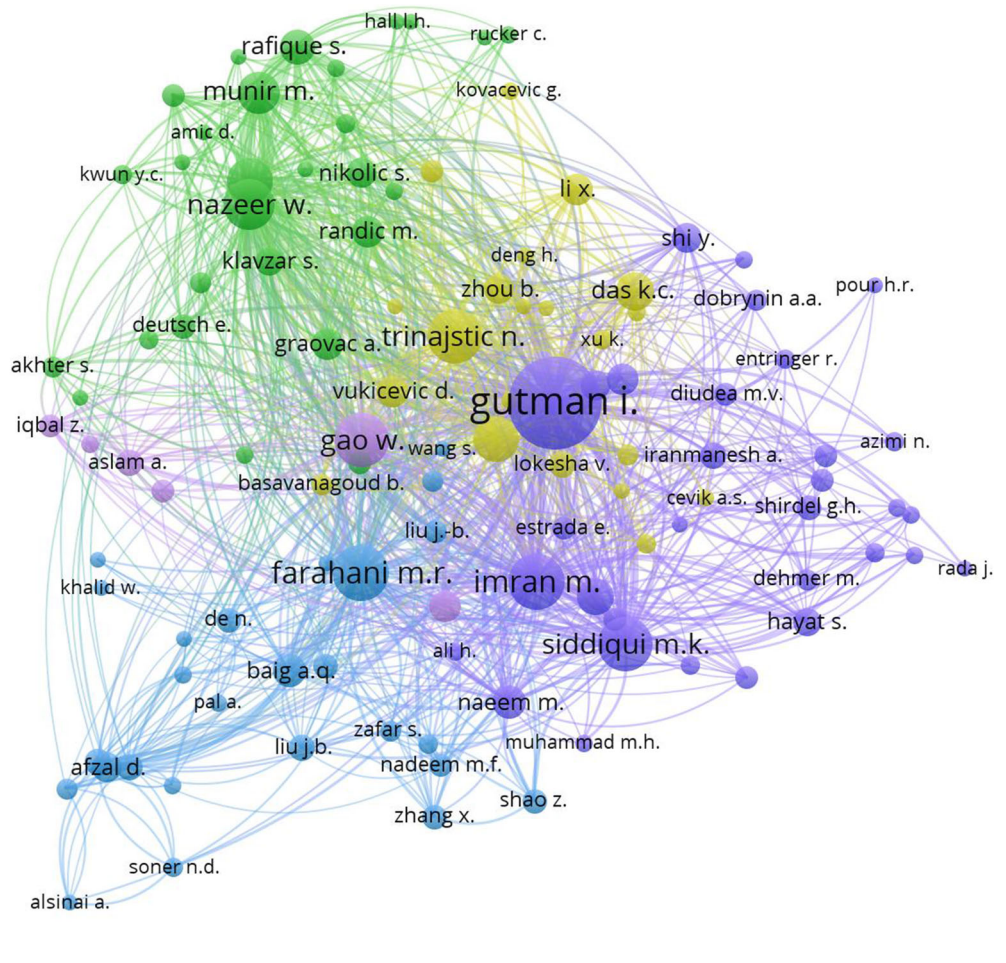
Using the edge partition from Table 1

$$= 2(9) + 2(10) + 2(12) + (2n - 2)(13) + 8(15) + 2(19) + 2(18) + (2n + 2)(21) + (n - 2)(12) + (n - 2)(22) + (6n - 12)(23) + (n - 2)(18),$$

we have got, by making some calculations

$$\implies M_1G_5(T) = 258n - 108.$$

□



**Fig. 3** Bibliometric analysis of  $M$ -polynomials by different authors

**Theorem 4.2** *The Superlattice structure,  $M_2G_5(T)$  corresponds to the fifth  $M$ -Zagreb index polynomial for a given graph*

$$M_2G_5(T) = 1317n - 990.$$

*Proof* Let  $T$  be the superlattice structure. Eq. (2) can be applied using this partition to

$$M_2G_5(T) = \sum_{uv \in E(T)} (\$T(u)\$T(v)),$$

Applying edge partition of Table 1

$$\begin{aligned} &= 2(18) + 2(21) + 2(36) + (2n - 2)(42) + 8(54) + 2(84) + 2(81) \\ &\quad + (2n + 2)(108) + (n - 2)(27) + (n - 2)(121) + (6n - 12)(132) + (n - 2)(77), \end{aligned}$$

we have got, by making some calculations

$$\implies M_2G_5(T) = 1317n - 990.$$

□

**Theorem 4.3** *Consider the Superlattice structure,  $M_1^aG_5(T)$  of fifth  $M$ -Zagreb index, polynomial for a structural graph, that is equal to:*

$$\begin{aligned} M_1^aG_5(T) &= 2(9)^a + 2(10)^a + 2(12)^a + (2n - 2)(13)^a + 8(15)^a \\ &\quad + 2(19)^a + 2(18)^a + (2n + 2)(21)^a + (n - 2)(12)^a \\ &\quad + (n - 2)(22)^a + (6n - 12)(23)^a + (n - 2)(18)^a \end{aligned}$$

**Table 1** Edge vertex degree based on superlattices

$(\S_T(u) : \S_T(v))$	Frequencies	$(\S_T(u) : \S_T(v))$	Frequencies
(3,6)	2	(9,9)	2
(3,7)	2	(9,12)	$2n + 2$
(6,6)	2	(3,9)	$n - 2$
(6,7)	$2n - 2$	(11,11)	$n - 2$
(6,9)	8	(11,12)	$6n - 12$
(7,12)	2	(11,7)	$n - 2$

*Proof* Let  $T$  be the Superlattice structure. From Eq. (3),

$$M_1^a G_5(T) = \sum_{uv \in E(T)} (\S_T(u) + \S_T(v))^a,$$

By implementing an edge partition on Table 1.

$$\begin{aligned} &= 2(3+6)^a + 2(3+7)^a + (2)(6+6)^a + (2n-2)(6+7)^a + 8(6+9)^a \\ &\quad + 2(7+12)^a + 2(9+9)^a + (2n+2)(9+12)^a + (n-2)(3+9)^a \\ &\quad + (n-2)(11+11)^a + (6n-12)(11+12)^a + (n-2)(11+7)^a, \end{aligned}$$

we have got, by making some calculations

$$\begin{aligned} \Rightarrow M_1^a G_5(T) &= 2(9)^a + 2(10)^a + 2(12)^a + (2n-2)(13)^a + 8(15)^a \\ &\quad + 2(19)^a + 2(18)^a + (2n+2)(21)^a + (n-2)(12)^a \\ &\quad + (n-2)(22)^a + (6n-12)(23)^a + (n-2)(18)^a \end{aligned}$$

□

**Theorem 4.4** Consider the Superlattice structure  $M_2^a G_5(T)$  of fifth  $M$ -Zagreb index as polynomial for a molecular graph, that is equal to:

$$\begin{aligned} M_2^a G_5(T) &= 2(18)^a + 2(21)^a + 2(36)^a + (2n-2)(42)^a + 8(54)^a \\ &\quad + 2(84)^a + 2(81)^a + (2n+2)(108)^a + (n-2)(27)^a \\ &\quad + (n-2)(121)^a + (6n-12)(132)^a + (n-2)(77)^a \end{aligned}$$

*Proof* Let  $T$  be the Superlattice structure. In Table 1, there is an frequency of  $T$ . From Eq. (4),

$$M_2^a G_5(T) = \sum_{uv \in E(T)} (\S_T(u)\S_T(v))^a,$$

Through the utilization of edge partitioning with respect to Table 1

$$\begin{aligned} &= 2(3 \times 6)^a + 2(3 \times 7)^a + (2)(6 \times 6)^a + (2n-2)(6 \times 7)^a + 8(6 \times 9)^a \\ &\quad + 2(7 \times 12)^a + 2(9 \times 9)^a + (2n+2)(9 \times 12)^a + (n-2)(3 \times 9)^a \\ &\quad + (n-2)(11 \times 11)^a + (6n-12)(11 \times 12)^a + (n-2)(11 \times 7)^a, \end{aligned}$$

we have got, by making some calculations

$$\begin{aligned} \Rightarrow M_2^a G_5(T) &= 2(18)^a + 2(21)^a + 2(36)^a + (2n-2)(42)^a + 8(54)^a \\ &\quad + 2(84)^a + 2(81)^a + (2n+2)(108)^a + (n-2)(27)^a \\ &\quad + (n-2)(121)^a + (6n-12)(132)^a + (n-2)(77)^a \end{aligned}$$

□

**Theorem 4.5** Consider the Superlattice structure  $HM_1 G_5(T)$  of fifth  $M$ -Zagreb index as polynomial for a chemical graph, that is equal to:

$$HM_1 G_5(T) = 5346n - 3888.$$

*Proof* Let  $T$  be the Superlattice structure. From Eq. (5),

$$HM_1G_5(T) = \sum_{uv \in E(T)} (\xi_T(u) + \xi_T(v))^2,$$

Through the use of Frequency as a means of partitioning table 1

$$\begin{aligned} &= 2(3 + 6)^2 + 2(3 + 7)^2 + (2)(6 + 6)^2 + (2n - 2)(6 + 7)^2 + 8(6 + 9)^2 \\ &\quad + 2(7 + 12)^2 + 2(9 + 9)^2 + (2n + 2)(9 + 12)^2 + (n - 2)(3 + 9)^2 \\ &\quad + (n - 2)(11 + 11)^2 + (6n - 12)(11 + 12)^2 + (n - 2)(11 + 7)^2, \end{aligned}$$

we have got, by making some calculations

$$\implies HM_1G_5(T) = 5346n - 3888.$$

□

**Theorem 4.6** Consider the Superlattice structure,  $HM_2G_5(T)$  of fifth  $M$ -Zagreb index, polynomial for a structural formula of graph is

$$HM_2G_5(T) = 152699n - 177202.$$

*Proof* Let  $T$  be the Superlattice structure. From Eq. (6),

$$HM_2G_5(T) = \sum_{uv \in E(T)} (\xi_T(u)\xi_T(v))^2,$$

By employing an edge partitioning technique on Table 1

$$\begin{aligned} &= 2(3 \times 6)^2 + 2(3 \times 7)^2 + (2)(6 \times 6)^2 + (2n - 2)(6 \times 7)^2 + 8(6 \times 9)^2 \\ &\quad + 2(7 \times 12)^2 + 2(9 \times 9)^2 + (2n + 2)(9 \times 12)^2 + (n - 2)(3 \times 9)^2 \\ &\quad + (n - 2)(11 \times 11)^2 + (6n - 12)(11 \times 12)^2 + (n - 2)(11 \times 7)^2 \end{aligned}$$

we have got, by making some calculations

$$\implies HM_2G_5(T) = 152699n - 177202.$$

□

**Theorem 4.7** Consider the Superlattice structure,  $M_3G_5(T)$  of fifth  $M$ -Zagreb index as polynomial for a molecular graph, that is equal to:

$$M_3G_5(T) = 21n + 46.$$

*Proof* Let  $T$  be the Superlattice structure. By Eq. (7),

$$M_3G_5(T) = \sum_{uv \in E(T)} |\xi_T(u) - \xi_T(v)|,$$

From Table 1

$$\begin{aligned} &= 2|3 - 6| + 2|3 - 7| + 2|6 - 6| + (2n - 2)|6 - 7| + 8|6 - 9| + 2|7 - 12| \\ &\quad + 2|9 - 9| + (2n + 2)|9 - 12| + (n - 2)|3 - 9| + (n - 2)|11 - 11| \\ &\quad + (6n - 12)|11 - 12| + (n - 2)|11 - 7|, \end{aligned}$$

we have got, by making some calculations

$$\implies M_3G_5(T) = 21n + 46.$$

□

**Theorem 4.8** Consider the Superlattice structure,  $M_1^aG_5(T, z)$  of fifth  $M$ -Zagreb index as polynomial, that is equal to:

$$\begin{aligned} M_1^aG_5(T, z) &= 2z^{(9)^a} + 2z^{(10)^a} + 2z^{(12)^a} + (2n - 2)z^{(13)^a} + 8z^{(15)^a} \\ &\quad + 2z^{(19)^a} + 2z^{(18)^a} + (2n + 2)z^{(21)^a} + (n - 2)z^{(12)^a} \\ &\quad + (n - 2)z^{(22)^a} + (6n - 12)z^{(23)^a} + (n - 2)z^{(18)^a} \end{aligned}$$

*Proof* Let  $T$  be the Superlattice structure. Using Eq. (8),

$$M_1^a G_5(T, z) = \sum_{uv \in E(T)} z^{(\delta_T(u) + \delta_T(v))^a}.$$

By implementing an edge-based partitioning strategy for Table 1

$$\begin{aligned} &= 2z^{(3+6)^a} + 2z^{(3+7)^a} + 2z^{(6+6)^a} + (2n-2)z^{(6+7)^a} + 8z^{(6+9)^a} \\ &\quad + 2z^{(7+12)^a} + 2z^{(9+9)^a} + (2n+2)z^{(9+12)^a} + (n-2)z^{(3+9)^a} \\ &\quad + (n-2)z^{(11+11)^a} + (6n-12)z^{(11+12)^a} + (n-2)z^{(11+7)^a} \end{aligned}$$

we have got, by making some calculations

$$\begin{aligned} \Rightarrow M_1^a G_5(T, z) &= 2z^{(9)^a} + 2z^{(10)^a} + 2z^{(12)^a} + (2n-2)z^{(13)^a} + 8z^{(15)^a} \\ &\quad + 2z^{(19)^a} + 2z^{(18)^a} + (2n+2)z^{(21)^a} + (n-2)z^{(12)^a} \\ &\quad + (n-2)z^{(22)^a} + (6n-12)z^{(23)^a} + (n-2)z^{(18)^a} \end{aligned}$$

□

**Theorem 4.9** Consider the Superlattice structure,  $M_2^a G_5(T, z)$  of fifth M-Zagreb index, polynomial for a structural formula of given graph, that is equal to [24]:

$$\begin{aligned} M_2^a G_5(T, z) &= 2z^{(18)^a} + 2z^{(21)^a} + 2z^{(36)^a} + (2n-2)z^{(42)^a} + 8z^{(54)^a} \\ &\quad + 2z^{(84)^a} + 2z^{(81)^a} + (2n+2)z^{(108)^a} + (n-2)z^{(27)^a} \\ &\quad + (n-2)z^{(121)^a} + (6n-12)z^{(132)^a} + (n-2)z^{(77)^a} \end{aligned}$$

*Proof* Let  $T$  be the Superlattice structure. From Eq. (9),

$$M_2^a G_5(T, z) = \sum_{uv \in E(T)} z^{(\delta_T(u)\delta_T(v))^a}.$$

Applying edge partition from Table 1

$$\begin{aligned} &= 2z^{(3 \times 6)^a} + 2z^{(3 \times 7)^a} + 2z^{(6 \times 6)^a} + (2n-2)z^{(6 \times 7)^a} + 8z^{(6 \times 9)^a} \\ &\quad + 2z^{(7 \times 12)^a} + 2z^{(9 \times 9)^a} + (2n+2)z^{(9 \times 12)^a} + (n-2)z^{(3 \times 9)^a} \\ &\quad + (n-2)z^{(11 \times 11)^a} + (6n-12)z^{(11 \times 12)^a} + (n-2)z^{(11 \times 7)^a} \end{aligned}$$

we have got, by making some calculations

$$\begin{aligned} \Rightarrow M_2^a G_5(T, z) &= 2z^{(18)^a} + 2z^{(21)^a} + 2z^{(36)^a} + (2n-2)z^{(42)^a} + 8z^{(54)^a} \\ &\quad + 2z^{(84)^a} + 2z^{(81)^a} + (2n+2)z^{(108)^a} + (n-2)z^{(27)^a} \\ &\quad + (n-2)z^{(121)^a} + (6n-12)z^{(132)^a} + (n-2)z^{(77)^a} \end{aligned}$$

□

**Theorem 4.10** Consider the Superlattice structure,  $M_1 G_5(T, z)$  of fifth M-Zagreb index as polynomial for given graph, equal to:

$$\begin{aligned} M_1 G_5(T, z) &= 2z^{(9)} + 2z^{(10)} + 2z^{(12)} + (2n-2)z^{(13)} + 8z^{(15)} \\ &\quad + 2z^{(19)} + 2z^{(18)} + (2n+2)z^{(21)} + (n-2)z^{(12)} \\ &\quad + (n-2)z^{(22)} + (6n-12)z^{(23)} + (n-2)z^{(18)} \end{aligned}$$



*Proof* Let  $T$  be the Superlattice structure. By Eq. (10),

$$M_1G_5(T, z) = \sum_{uv \in E(T)} z^{\$T(u)+\$T(v)}.$$

From Edge segmentation of  $T$  Table 1

$$\begin{aligned} &= 2z^{(3+6)} + 2z^{(3+7)} + 2z^{(6+6)} + (2n - 2)z^{(6+7)} + 8z^{(6+9)} \\ &\quad + 2z^{(7+12)} + 2z^{(9+9)} + (2n + 2)z^{(9+12)} + (n - 2)z^{(3+9)} \\ &\quad + (n - 2)z^{(11+11)} + (6n - 12)z^{(11+12)} + (n - 2)z^{(11+7)} \end{aligned}$$

we have got, by making some calculations

$$\begin{aligned} \Rightarrow M_1G_5(T, z) &= 2z^{(9)} + 2z^{(10)} + 2z^{(12)} + (2n - 2)z^{(13)} + 8z^{(15)} \\ &\quad + 2z^{(19)} + 2z^{(18)} + (2n + 2)z^{(21)} + (n - 2)z^{(12)} \\ &\quad + (n - 2)z^{(22)} + (6n - 12)z^{(23)} + (n - 2)z^{(18)} \end{aligned}$$

□

**Theorem 4.11** Consider the Superlattice structure,  $M_2G_5(T, z)$  of fifth  $M$ -Zagreb index polynomial for a chemical graph, that is equal to:

$$\begin{aligned} M_2G_5(T, z) &= 2z^{(18)} + 2z^{(21)} + 2z^{(36)} + (2n - 2)z^{(42)} + 8z^{(54)} \\ &\quad + 2z^{(84)} + 2z^{(81)} + (2n + 2)z^{(108)} + (n - 2)z^{(27)} \\ &\quad + (n - 2)z^{(121)} + (6n - 12)z^{(132)} + (n - 2)z^{(77)} \end{aligned}$$

*Proof* Let  $T$  be the Superlattice structure. Through Eq. (11),

$$M_2G_5(T, z) = \sum_{uv \in E(T)} z^{\$T(u)\$T(v)}.$$

By use of Table 1

$$\begin{aligned} &= 2z^{(3 \times 6)} + 2z^{(3 \times 7)} + 2z^{(6 \times 6)} + (2n - 2)z^{(6 \times 7)} + 8z^{(6 \times 9)} \\ &\quad + 2z^{(7 \times 12)} + 2z^{(9 \times 9)} + (2n + 2)z^{(9 \times 12)} + (n - 2)z^{(3 \times 9)} \\ &\quad + (n - 2)z^{(11 \times 11)} + (6n - 12)z^{(11 \times 12)} + (n - 2)z^{(11 \times 7)} \end{aligned}$$

we have got, by making some calculations

$$\begin{aligned} \Rightarrow M_2G_5(T, z) &= 2z^{(18)} + 2z^{(21)} + 2z^{(36)} + (2n - 2)z^{(42)} + 8z^{(54)} \\ &\quad + 2z^{(84)} + 2z^{(81)} + (2n + 2)z^{(108)} + (n - 2)z^{(27)} \\ &\quad + (n - 2)z^{(121)} + (6n - 12)z^{(132)} + (n - 2)z^{(77)} \end{aligned}$$

□

**Theorem 4.12** Consider the Superlattice structure,  $M_1G_5(T, z)$  of fifth  $M$ -Zagreb index as polynomial for a chemical graph, that is equal to:

$$\begin{aligned} M_1G_5(T, z) &= 2z^{(81)} + 2z^{(100)} + 2z^{(144)} + (2n - 2)z^{(169)} + 8z^{(225)} \\ &\quad + 2z^{(361)} + 2z^{(324)} + (2n + 2)z^{(441)} + (n - 2)z^{(144)} \\ &\quad + (n - 2)z^{(484)} + (6n - 12)z^{(529)} + (n - 2)z^{(324)} \end{aligned}$$

*Proof* Let  $T$  be the Superlattice structure. From Eq. (12),

$$M_1 G_5(T, z) = \sum_{uv \in E(T)} z^{(\delta_T(u) + \delta_T(v))^2}.$$

By applying the concept of edge frequency to Table 1.

$$\begin{aligned} &= 2z^{(3+6)^2} + 2z^{(3+7)^2} + 2z^{(6+6)^2} + (2n-2)z^{(6+7)^2} + 8z^{(6+9)^2} \\ &\quad + 2z^{(7+12)^2} + 2z^{(9+9)^2} + (2n+2)z^{(9+12)^2} + (n-2)z^{(3+9)^2} \\ &\quad + (n-2)z^{(11+11)^2} + (6n-12)z^{(11+12)^2} + (n-2)z^{(11+7)^2} \end{aligned}$$

we have got, by making some calculations

$$\begin{aligned} \Rightarrow M_1 G_5(T, z) &= 2z^{(81)} + 2z^{(100)} + 2z^{(144)} + (2n-2)z^{(169)} + 8z^{(225)} \\ &\quad + 2z^{(361)} + 2z^{(324)} + (2n+2)z^{(441)} + (n-2)z^{(144)} \\ &\quad + (n-2)z^{(484)} + (6n-12)z^{(529)} + (n-2)z^{(324)} \end{aligned}$$

□

**Theorem 4.13** Consider the Superlattice structure,  $M_2 G_5(T, z)$  of fifth  $M$ -Zagreb index polynomial for a molecular graph, which is equal to:

$$\begin{aligned} M_2 G_5(T, z) &= 2z^{(324)} + 2z^{(441)} + 2z^{(1296)} + (2n-2)z^{(1764)} + 8z^{(2916)} \\ &\quad + 2z^{(7056)} + 2z^{(6561)} + (2n+2)z^{(11664)} + (n-2)z^{(729)} \\ &\quad + (n-2)z^{(14641)} + (6n-12)z^{(17424)} + (n-2)z^{(5929)} \end{aligned}$$

*Proof* Let  $T$  be the Superlattice structure. From Eq. (13),

$$M_2 G_5(T, z) = \sum_{uv \in E(T)} z^{(\delta_T(u)\delta_T(v))^2}.$$

Through Table 1.

$$\begin{aligned} &= 2z^{(3 \times 6)^2} + 2z^{(3 \times 7)^2} + 2z^{(6 \times 6)^2} + (2n-2)z^{(6 \times 7)^2} + 8z^{(6 \times 9)^2} \\ &\quad + 2z^{(7 \times 12)^2} + 2z^{(9 \times 9)^2} + (2n+2)z^{(9 \times 12)^2} + (n-2)z^{(3 \times 9)^2} \\ &\quad + (n-2)z^{(11 \times 11)^2} + (6n-12)z^{(11 \times 12)^2} + (n-2)z^{(11 \times 7)^2} \end{aligned}$$

we have got, by making some calculations

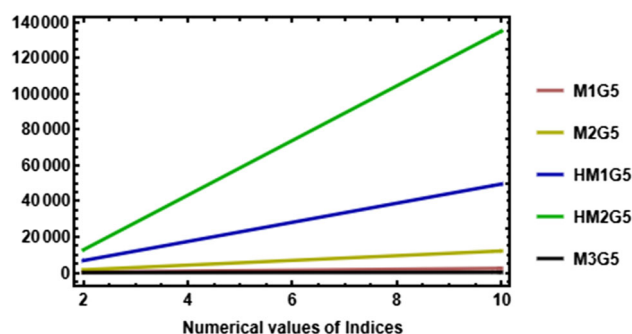
$$\begin{aligned} \Rightarrow M_2 G_5(T, z) &= 2z^{(324)} + 2z^{(441)} + 2z^{(1296)} + (2n-2)z^{(1764)} + 8z^{(2916)} + \\ &\quad 2z^{(7056)} + 2z^{(6561)} + (2n+2)z^{(11664)} + (n-2)z^{(729)} + \\ &\quad (n-2)z^{(14641)} + (6n-12)z^{(17424)} + (n-2)z^{(5929)} \end{aligned}$$

□

The numerical and graphical representation if above computed results are depicted in Table 2 and Fig. 4, respectively.

**Table 2** The Fifth Zagreb Indices, both general and degree-based of Superlattice Network for  $n = 1$  to 10 with comparison of numbers

n	$M_1G_5(T)$	$M_2G_5(T)$	$M_3G_5(T)$	$HM_2G_5(T)$	$HM_1G_5(T)$
1	150	327	67	1458	-24503
2	408	1644	88	6804	128196
3	666	2961	109	12150	280895
4	924	4278	130	17496	433594
5	1182	5595	151	22842	586293
6	1440	6912	172	28188	738992
7	1698	8229	193	33534	891691
8	1956	9546	214	38880	1044390
9	2214	10863	235	44226	1197089
10	2472	12180	256	49572	1349788

**Fig. 4** Numerical values of indices

## 5 Conclusion

In this paper, the analysis of superlattice structure with the help of fifth  $M$ -Zagreb polynomials and fifth  $M$ -Zagreb indices provides a deeper understanding of the structural and chemical and physical properties i. e such as boiling and melting points, refractive index, and dielectric constant of the superlattice. The fifth  $M$ -Zagreb polynomials and indices provide a quantitative measure of the degree of branching of the molecules in the superlattice. Using the fifth  $M$ -Zagreb polynomials and indices can provide valuable insights into the degree of branching and topological properties of the material.

**Funding** This research received no funding.

**Data availability** In this article, no data were utilized.

## Declarations

**Conflict of interest** Authors have no conflict of interest.

## References

1. A. Al Khabyah, Mathematical aspects and topological properties of two chemical networks. *AIMS Mathematics* **8**(2), 4666–4681 (2023)
2. H. Ali, M.A. Binyamin, M.K. Shafiq, W. Gao, On the degree-based topological indices of some derived networks. *Mathematics* **7**(7), 6–12 (2019)
3. A. Ali, M. Zahid, W. Gao, M. Imran, Topological indices and cheminformatics applications. *Mol. Sci.* **22**(6), 30–96 (2021)
4. D. Amic, D. Beslo, B. Lucic, S. Nikolic, N. Trinajstic, The vertex-connectivity index revisited. *J. Chem. Inf. Comput. Sci.* **38**(5), 819–822 (1998)
5. M. Ali, A. Latif, S. Gao, K. Mahmood, QSPR modeling of boiling point of organic compounds using topological indices. *Mol. Liq.* **279**, 177–184 (2019)
6. M. Eliasi, A. Iranmanesh, I. Gutman, Multiplicative versions of first Zagreb index. *Match-Commun. Math. Comput. Chem.* **68**(1), 2–17 (2012)
7. B. Furtula, A. Graovac, Novel vertex-weighted molecular topological indices. *J. Comput. Chem.* **32**(12), 2726–2739 (2011)
8. I. Gutman, N. Trinajstic, Graph theory and molecular orbitals. Total  $\pi$ -electron energy of alternant hydrocarbons. *Chem. Phys. Lett.* **17**(4), 535–538 (1972)
9. Xiujun Zhang, Hafiz Muhammad Awais, Muhammad Javaid, Muhammad Kamran Siddiqui, Multiplicative Zagreb indices of molecular graphs. *J. Chem.* **2019**, 1–19 (2019)
10. X. Zhang, H. Jiang, J.B. Liu, Z. Shao, The cartesian product and join graphs on edge-version atom-bond connectivity and geometric arithmetic indices. *Molecules* **23**(7), 17–31 (2018)
11. Z. Shao, M.K. Siddiqui, M.H. Muhammad, Computing Zagreb indices and Zagreb polynomials for symmetrical nanotubes. *Symmetry* **10**(7), 244–260 (2018)

12. W. Gao, M.K. Siddiqui, M. Naeem, N.A. Rehman, Topological characterization of carbon graphite and crystal cubic carbon structures. *Molecules* **22**(9), 1496–1515 (2017)
13. X. Zhang, A. Rauf, M. Ishtiaq, M.K. Siddiqui, M.H. Muhammad, On degree based topological properties of two carbon nanotubes. *Polycyclic Aromat. Compd.* **42**(3), 866–884 (2022)
14. X. Zhang, M. Naeem, A.Q. Baig, M.A. Zahid, Study of hardness of superhard crystals by topological indices. *J. Chem.* **2021**, 1–10 (2021)
15. X. Zhang, M.K. Siddiqui, S. Javed, L. Sherin, F. Kausar, M.H. Muhammad, Physical analysis of heat for formation and entropy of Ceria Oxide using topological indices. *Combinatorial Chem. High Throughput Screen.* **25**(3), 441–450 (2022)
16. X. Zhang, Z. Zhang, N. Chidambaram, S. Jaganathan, N. Devadoss, V. Ravi, On degree and distance-based topological indices of certain interconnection networks. *Eur. Phys. J. Plus* **137**(7), 1–15 (2022)
17. I. Gutman, Degree-based topological indices. *Croat. Chem. Acta* **86**(4), 351–361 (2013)
18. I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. XIII. On the stability of annelated tropylium cations. *Croat. Chem. Acta* **46**(4), 243–248 (1974)
19. I. Gutman, Multiplicative Zagreb indices of trees. *Bull. Soc. Math. Banja Luka* **18**, 17–23 (2011)
20. M. Ghorbani, A.R. Ashrafi, S.R. Pour, Some new degree-based topological indices. *Comput. Chem.* **39**(28), 2444–2455 (2018)
21. A. Graovac, M. Ghorbani, M.A. Hosseinzadeh, Computing fifth geometric-arithmetic index for nanostar dendrimers. *J. Discret. Math. Appl.* **1**(1–2), 33–42 (2011)
22. R. Huang, M.H. Muhammad, M.K. Siddiqui, S. Khalid, S. Manzoor, E. Bashier, Analysis of topological aspects for metal-insulator transition superlattice network. *Complexity* **10**, 1–12 (2022)
23. V.R. Kulli, Multiplicative hyper-Zagreb indices and coindices of graphs: computing these indices of some nanostructures. *Int. Res. J. Pure Algebra* **6**(7), 342–347 (2016)
24. V.R. Kulli, General fifth M-Zagreb indices and fifth M-Zagreb polynomials of PAMAM dendrimers. *Int. J. Fuzzy Math. Arch.* **13**(1), 99–103 (2017)
25. V.R. Kulli, B. Chaluvaram, T.V. Asha, Multiplicative product connectivity and sum connectivity indices of chemical structures in drugs. *Res. Rev. Int. J. Multidiscip.* **4**(2), 949–953 (2019)
26. V.R. Kulli, HDR Zagreb indices of remdesivir, chloroquine, hydroxychloroquine: research for the treatment of COVID-19. *SSRG Int. J. Appl. Chem.* **9**(1), 1–9 (2022)
27. W. Liu, Z. Zhu, K. Cai, D. Pu, Y. Du, Application of knowledge graph in smart grid fault diagnosis. *Appl. Math. Nonlinear Sci.* (2022)
28. J. Lu, L. Zhu, W. Gao, Remarks on bipolar cubic fuzzy graphs and its chemical applications. *Int. J. Math. Comput. Eng.* **1**(1), 1–10 (2023)
29. L. Ma, C. Dou, T. Hao, Grid data asset relationship and intelligent classification integrating knowledge graph and Internet of Things. *Appl. Math. Nonlinear Sci.* **24**(5), 328–340
30. S. Nagarajan, M. Imran, P.M. Kumar, K. Pattabiraman, M.U. Ghani, Degree-based entropy of some classes of networks. *Mathematics* **11**(4), 960–967 (2023)
31. S. Raoux, W. Welnic, D. Ielmini, Phase change materials and their application to nonvolatile memories. *Chem. Rev.* **110**(1), 240–267 (2010)
32. V.K. Sharma, S. Sharma, A.K. Madan, A review on distance-based topological indices in quantitative structure activity relationship. *Comput. Chem.* **40**(8), 839–876 (2019)
33. R.E. Simpson, P. Fons, A.V. Kolobov, T. Fukaya, M. Krbal, S. Yagi, Disorder-order phase transition in GeSbTe. *Appl. Phys.* **109**(10), 1024–1040 (2011)
34. Y. Wu, F. Lv, M. Li, The application of graph theory teaching method in ideological and political education of discrete mathematics. *Appl. Math. Nonlinear Sci.* **39**(6), 8125–8137

Springer Nature or its licensor (e.g. a society or other partner) holds exclusive rights to this article under a publishing agreement with the author(s) or other rightsholder(s); author self-archiving of the accepted manuscript version of this article is solely governed by the terms of such publishing agreement and applicable law.