Journal of Discrete Mathematical Sciences & Cryptography
ISSN 0972-0529 (Print), ISSN 2169-0065 (Online)
Vol. 29 (2026), No. 7, pp. 2963–2976
DOI : 10.47974/JDMSC-2456

Topological analysis of the molecular graph of monolayer $M_3C_{12}X_{12}$ Kagome structures using degree-based indices

Mohammad Reza Farahani [†]
Mehdi Alaeiyan [*]
School of Mathematics and Computer Science
Iran University of Science & Technology (IUST)
Narmak 16844
Tehran
Iran

Muhammad Shoaib Sardar [§]
School of Mathematical Sciences
Harbin Engineering University
Nangang District
Harbin 150001
China

Shobha V. Patil [‡]
Department of Mathematics
Dr. M. S. Sheshgiri College of Engineering and Technology
KLE Technological University
Belagavi 590001
Karnataka
India

[†] *ORCID-ID:* **0000-0003-2969-4280**
[*] *ORCID-ID:* **0000-0003-2185-5967**
[§] *ORCID-ID:* **0000-0001-7146-5639**
[‡] *ORCID-ID:* **0000-0002-6210-832X**

[†] *E-mail:* **mohammad_farahani@mathdep.iust.ac.ir; mrfarhani88@gmail.com**
[*] *E-mail:* **alaeiyan@iust.ac.ir (Corresponding Author)**
[§] *E-mail:* **shoaibsardar093@gmail.com**
[‡] *E-mail:* **shobhap49@gmail.com**

Murat Cancan [@]
Department of Mathematics
Faculty of Education
Yuzuncu Yil University
Van 65090
Turkey

Abstract

Two-dimensional (2D) magnetic materials have arisen as viable contenders for next-generation nano-spintronics, quantum computing and high-density data storage technologies, owing to their distinctive magnetic and electrical characteristics at the atomic level. This study examines the molecular graph of a two-dimensional monolayer structure M3C12X12, where M represents a metal atom, C signifies carbon and X indicates a halogen atom. The molecule displays a Kagome lattice configuration, recognised for its unusual electrical properties. Employing graph-theoretic methodologies, we calculate several degree-based topological indices, such as the First Zagreb index, First hyper-Zagreb index, First and Second Gourava indices, Reciprocal Randic index, First and Second K-Banhatti indices and the Platt index. These indices function as molecular descriptors that measure structural characteristics pertinent to the compound's physicochemical and magnetic properties. Our work illustrates the efficacy of topological indices in the structural characterisation of 2D materials and establishes a basis for further theoretical and computational investigations in materials science and nano-technology.

Subject Classification: *05C92.*

Keywords: *$M_3C_{12}X_{12}$ lattice, Chemical graph, QSAR, QSPR, Topological descriptors.*

1. Introduction

Two-dimensional (2D) magnetic materials have garnered considerable interest owing to their potential applications in burgeoning domains such as nano-spintronics, quantum information processing and highdensity data storage technologies [1, 2]. These materials demonstrate distinctive magnetic, electrical and structural characteristics at the atomic level, rendering them optimal candidates for next-generation electronics. Half-metallic (HM) magnets are particularly noteworthy due to their possible application in spin-filters, which facilitate the formation of a completely spin-polarized current, hence promoting low energy consumption and enhancing the performance of spintronic devices [2, 3]. Moreover,

[@] *ORCID-ID:* **0000-0002-8606-2274**

[@] *E-mail:* **mcancan@yyu.edu.tr**

ferromagnetic semiconductors, such as bipolar magnetic semiconductors (BMSs), are considered attractive prospects for effective spin production and injection methods in spintronic technologies.

However, there are a number of basic problems that make it hard for these materials to be widely used. These include the need for high Curie temperatures, high saturation magnetisation, high magnetic anisotropy energies and long-range magnetic order. The exploration of novel 2D materials with tailored magnetic and structural attributes continues to be an active area of study to address these challenges.

In this study, we focus on the molecular graph corresponding to the monolayer lattice structure of $M_3C_{12}X_{12}$, where M signifies a metal atom, C indicates carbon and X denotes a halogen atom. This chemical makes a 2D Kagome lattice out of corner-sharing equilateral triangles. This shape is famous for its unusual electrical and magnetic characteristics, such Dirac cones and flat bands. The distinctive symmetry and connectivity of this lattice structure have motivated researchers to explore several 2D metalorganic framework (MOF) possibilities that share analogous topologies. They are especially interested in the candidates' inherent magnetic and electronic characteristics, which are being studied using firstprinciples calculations and theoretical analysis.

Since the discovery of graphene [4], there has been a lot of interest in 2D covalent-organic frameworks and layered nanostructures because of their unique physical properties and their use in small electronic parts. Numerous studies have been conducted on 2D boron nitride nanomeshes [7], metal carbides [8], graphene oxide [9], silicene [10], porous graphene [11], and molybdenum disulphide (MoS_2) [12] for a wide range of uses. The continuous search for innovative 2D materials is crucial to meet the growing demands in materials science and nanotechnology [5, 6, 8]. Simultaneously, there has been substantial progress in the synthesis and use of metal-organic frameworks (MOFs), which have exhibited considerable promise in several domains, including drug delivery, sensing, gas storage and catalysiscitere [13, 14]. MOFs are porous materials formed by the coordination of metal ions or clusters with organic ligands. This unique structure gives them several advantages, including a large surface area, tunable pore size and diverse functionality.

Graph-theoretic techniques have shown to be exceptionally helpful in examining the structural characteristics of these molecular lattices. A molecular graph is a mathematical idea in which atoms are shown as vertices and chemical bonds as edges. Topological indices, which are numerical invariants that come from these networks, are very useful for

linking structure information to several physicochemical and biological aspects of the substance. Degree-based topological indices have been extensively utilised in modelling quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) within cheminformatics, drug design, nanomaterials characterisation and toxicity prediction [15].

This study analyses the calculation of diverse degree-based topological indices for the molecular graph of the $M_3C_{12}X_{12}$ monolayer. The indexes include the First Zagreb index, the First hyper-Zagreb index, the First and Second Gourava indices, the Reciprocal Randic index, the First and Second K-Banhatti indices and the Platt index. Prior graph-theoretic studies have been conducted on molecular structures, encompassing Alzheimer drug compounds [15], silicon carbide [16], and alkane structures [17], demonstrating the versatility and efficacy of topological indices in the examination of diverse molecular systems.

The rest of this work is set up like this: Section 2 outlines the necessary prerequisites and formal definitions of the topological indices studied in this work. Section 3 shows what we found in our study, along with graphs and a full explanation. In the conclusion, Section 4 finishes the study and talks about what could happen in the future.

2. Molecular Graph Structure and Topological Indices

2.1 *The $M_3C_{12}X_{12}$ Lattice Structure*

The $M_3C_{12}X_{12}$ lattice is a two-dimensional molecular structure where *M* stands for metal atoms, *C* stands for carbon atoms and *X* stands for halogen atoms. The numbers below each letter show how many of each type of atom there are. This lattice has a kagome-like structure, with atoms arranged in a hexagonal framework and alternating metal and carbon-halogen connections [18-23].

The atomic structure may be shown as a molecular graph $G=(V(G),E(G))$, where vertices represent atoms and edges indicate chemical bonds. The $M_3C_{12}X_{12}(m,n)$ extension of this lattice, which has $m\times n$ unit cells, has $54mn-25m-25n+25$ *vertices and* $72mn-36m-36n+36$ *edges. to unit cells, has* $29mn-(n-1)-n(m-1)=27mn+m+n$ *vertices and* $36mn$ *edges.*

Figure 1 shows this structure, which might be used in quantum computing and spintronics because of its unique electrical properties.

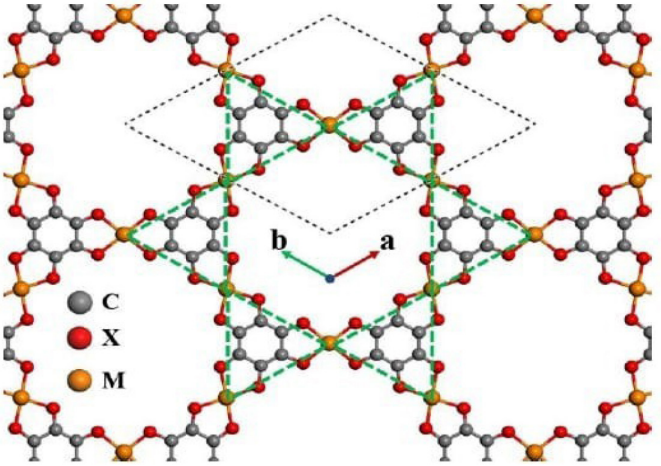


Figure 1

The molecular graph of $M_3C_{12}X_{12}$ lattice.

2.2 *Graph Theoretical Foundations*

A molecular graph is a simple graph (no loops or multiple edges) where:

- The degree d_v of vertex v enumerates its incident edges (chemical bonds).
- Topological indices are numerical representations that remain unchanged under graph isomorphism.
- These indices represent molecular characteristics in QSAR/QSPR analyses.

2.3 *Degree-Based Topological Indices*

We analyze the $M_3C_{12}X_{12}$ lattice using these indices in Table 1:

Table 1

Key topological indices and their chemical significance.

Degree-Based Topological Indices	Chemical Interpretation
First hyper-Zagreb (HM_1)	Degree variance between adjacent atoms
Gourava indices ($GO1.GO_2$)	Combined additive/multiplicative bond effects
Reciprocal Randic (RR)	Molecular branching and connectivity
K-Banhatti ($B_1.B_2$)	Vertex-edge interactions in bonding networks
Platt (Pl)	Molecular cyclicity and strain
Zagreb (M_1)	Total bond energy approximation

Mathematically, these indices are defined as:

$$HM_1(G) = \sum_{uv \in E(G)} (d_u + d_v)^2, GO_1(G) = \sum_{uv \in E(G)} (d_u + d_v + d_u d_v), GO_2(G) = \sum_{uv \in E(G)} (d_u + d_v) d_u d_v,$$

$$RR(G) = \sum_{uv \in E(G)} \sqrt{d_u d_v}, B_1(G) = \sum_{uv \in E(G)} (3d_u + 3d_v - 4), B_2(G) = \sum_{uv \in E(G)} (d_u + d_v)(d_u + d_v - 2),$$

$$Pl(G) = M_1(G) - 2|E(G)| \quad \text{where} \quad M_1(G) = \sum_{v \in V(G)} d_v^2$$

2.4 *Computational Approach*

For the $M_3C_{12}X_{12}(m,n)$ lattice, we:

1. Classify edges by vertex degree pairs (d_u, d_v)
2. Derive general formulas for each index
3. Analyze trends using 3D plots and heatmaps (Figure 3 (a)-3 (p))
4. Growth of various topological indices with respect to the parameter $m=n$.

3. Main Results

3.1 *Structural Analysis and Edge Partitioning*

The molecular graph of $M_3C_{12}X_{12}(m,n)$ (Figure 1) contains vertices with degrees 2, 3 and 4, which generate distinct edge types that are essential for the computation of the topological index. The complete edge partitioning is illustrated in Table 2, which serves as the basis for our analytical approach.

Table 2

Edge partitioning of $M_3C_{12}X_{12}$ lattice based on vertex degrees.

(d_u, d_v) where $uv \in E(M_3C_{12}X_{12}(m,n))$	Number of edges
(2, 2)	(4m+4n)
(2, 3)	(12mn)
(2, 4)	(12mn-4m-4n)
(3, 3)	(12mn)

3.2 *Computational Framework*

We developed a systematic algorithm (Algorithm **D-TI**) for computing topological indices that combines:

- Degree-based edge partition data from Table 2
- Mathematical formulations of each index
- Cross-verification through index relationships (e.g., Platt-Zagreb identity)

Algorithmic Details: The computation involves three phases:

1. **Initialization**: Set all index accumulators to zero
2. **Edge Processing:** For each edge type (d_u,d_v), compute: $s=d_u+d_v$ (degree sum), $p=d_{u\times}d_v$ (degree product) and Update each index using its specific formula
3. Validation: Verify consistency between direct Platt calculation and Zagreb-derived value Ensure edge count matches theoretical prediction (See Algorithm 1).

Algorithm 1 Computation of Degree-Based Topological Indices (D-TI)

Algorithm 1 Computation of Degree-Based Topological Indices (D-TI)

Require: Edge partition $\{(d_u, d_v) \mapsto f_{d_u,d_v}(m,n)\}$ of $G = M_3C_{12}X_{12}$
Ensure: Symbolic expressions for all indices
Initialize accumulators: $HM_1, GO_1, \ldots, M_1 \leftarrow 0$
$|E| \leftarrow 0$ ▷ Total edge counter
for all edge types (d_u, d_v) with count $f_{d_u,d_v}(m,n)$ **do**
  Compute $s = d_u + d_v$, $p = d_u \cdot d_v$
  $HM_1 \leftarrow HM_1 + f_{d_u,d_v}(m,n) \cdot s^2$
  $GO_1 \leftarrow GO_1 + f_{d_u,d_v}(m,n) \cdot (s+p)$
  ⋮ ▷ Similar updates for other indices
  $|E| \leftarrow |E| + f_{d_u,d_v}(m,n)$
end for
Verify $Pl(G) \stackrel{?}{=} M_1(G) - 2|E|$
return Index polynomials in (m,n)

1.1 *Closed-Form Solutions*

Applying Algorithm **D-TI** yields exact expressions for each index:

$GO_1(G)=480mn-32m-32n.$

$GO_2(G)=1584mn-128m-128n.$

B1(G)=468mn-24m-24n.

B2(G)=756mn-64m-64n.

Pl(Ω(m,n))= 204mn-8m-8n-36mn=168mn-8m-8n.

M1(G)=204mn-8m-8n.

Discussion. The topological descriptors are influenced by the structural parameters m and n of $M_3C_{12}X_{12}$, as indicated by these symbolic expressions:

- The term mn is the primary factor contributing to the indexes' growth, which is indicative of the molecule's recurrent modular structure.
- The **First hyper-Zagreb index** (HM_1) and **Second Gourava index** (GO_2) demonstrate the most rapid growth rates, rendering them susceptible to molecular expansion and branching.
- **The Reciprocal Randic index** is sensitive to nonuniform degree pairings, such as (2,3) and (2,4), as evidenced by the presence of irrational elements involving $\sqrt{6}$ and $\sqrt{2}$.
- The internal consistency of our results and the correctness of the D-TI Algorithm are confirmed by the accurate matching of the **Platt index** computed directly and via the Zagreb identity (modulo symbolic simplification).
- Although both **K Banhatti indices** scale similarly to the Zagreb-type indices, they include adjusted degree-based edge contributions that are beneficial for comparative molecular stability analysis.

These formulae, derived using the D-TI Algorithm, can be used to analyze and compare structural features of related molecular networks or substituted derivatives of $M_3C_{12}X_{12}$.

Graphical Analysis of Topological Indices

In order to acquire a more comprehensive understanding of the structural behaviour of $M_3C_{12}X_{12}$, we assessed the closed-form expressions of the topological indices for a range of m and n. The growth trends and mutual comparisons of the indices were analysed by plotting them as functions of m and n. The sensitivity of each index to changes in molecular complexity is exemplified by these graphical analyses, which also verify the symbolic trends that were obtained through the D-TI Algorithm.

In order to compare the asymptotic growth of various topological indices in the molecular graph

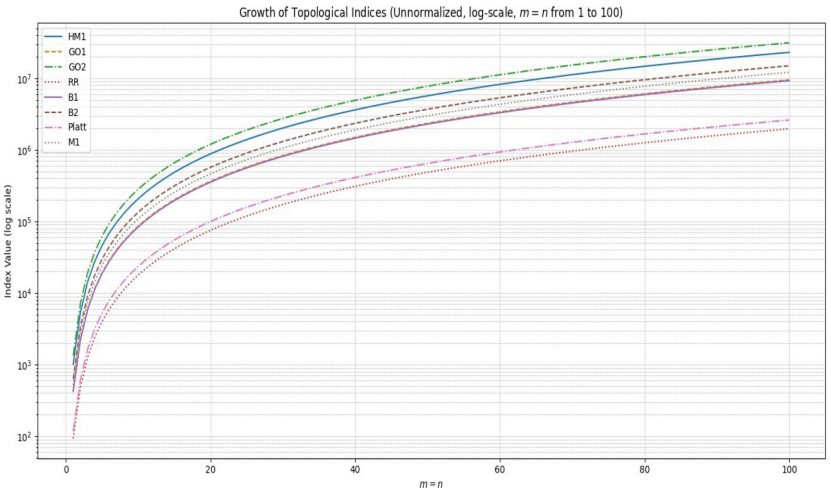


Figure 2

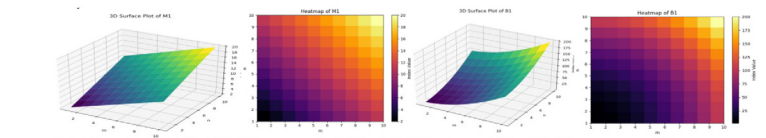
Growth of various topological indices with respect to the parameter m=n in the $M_3C_{12}X_{12}$. The indices are plotted without normalization on a logarithmic scale to emphasize their asymptotic behavior.

$M_3C_{12}X_{12}$, we assessed each index for values of m=n that ranged from 1 to 100. The results are presented on a logarithmic scale in Figure 2, which demonstrates a significant degree of variation in the magnitude and rate of increase among the indices. In particular, the second geometric-arithmetic index (GO_2) and the hyper-Zagreb index (HM_1) demonstrate the most rapid development, with the forgotten index (F), the first and second bond incident degree indices (B_1,B_2) and the Randic-Rouvray (RR) index being closely followed. In the interim, the Platt index and the initial Zagreb index (M_1) expand at a significantly slowed pace.

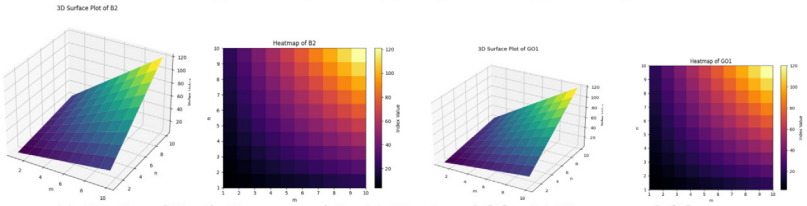
This necessitates the utilisation of a logarithmic y-axis, as it emphasises scaling disparities that are not readily evident when the indices are normalised over a restricted range. This plot illustrates that the comparative magnitudes of all indices are significantly influenced by the presence of nonlinear elements (such as square roots) and the leading coefficients, despite the fact that they all grow polynomially with respect to the network size. These discoveries provide a profound insight into the indexes' responsiveness to the graph structure and validate their use in characterising diverse silicate network attributes.

3.4 *3D surface plots*

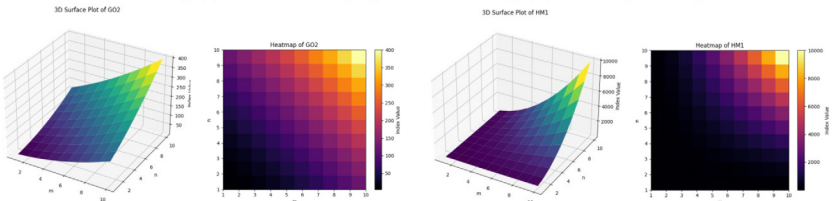
The lattice measuring $M_3C_{12}X_{12}$ underwent calculation and examination of its topological indices. Figures 3 (a) to 3 (p) show the three-dimensional surface plots and heatmaps for each of the sixteen indices that we are interested in. The goal of this section is to show eight topological indices in a visual way using three-dimensional surface plots and the heatmaps that go with it. Figures 3 (a) to 3 (p) show these pictures. Each index is shown with two graphs. The first plot is a three-dimensional surface plot that shows how the index values vary based on the parameters m and n. The second plot is a heatmap, which shows the same data in two dimensions with colour coding to make it easier to understand and compare. These visualisations show the patterns of growth, trends and symmetry that go along with the numbers when the graph parameters are



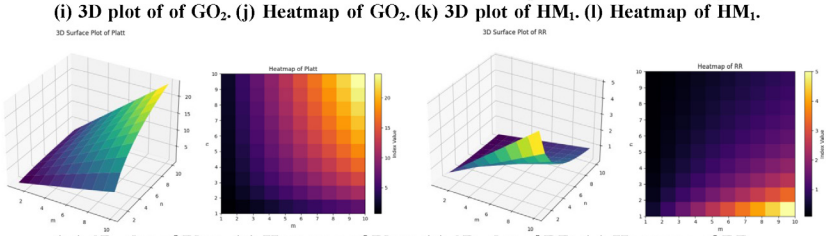
(a) 3D plot of M_1. (b) Heatmap of M_1. (c) 3D plot of B_1. (d) Heatmap of B_1.



(e) 3D plot of B_2. (f) Heatmap of B_2. (g) 3D plot of GO_1. (h) Heatmap of GO_1.



(i) 3D plot of of GO_2. (j) Heatmap of GO_2. (k) 3D plot of HM_1. (l) Heatmap of HM_1.



(m) 3D plot of Platt. (n) Heatmap of Platt. (o) 3D plot of RR. (p) Heatmap of RR.

Figure 3

Topological indices of $M_3C_{12}X_{12}$ lattice: (a-P).

changed. To understand how the graphs, work and how sensitive and discriminating each index is, you need to have these types of insights. You may use these charts to understand and compare the mathematical and chemical meanings of the topological indices. This makes them a highly helpful tool. This shows how the indices change in both variables in a way that you can see.

4. Conclusion

This study investigates the molecular graph associated with the monolayer lattice structure of $M_3C_{12}X_{12}$, a two-dimensional metal-organic framework (MOF) characterised by a Kagome lattice topology, recognised for its fascinating magnetic and electronic characteristics. Utilising graph-theoretic methodologies, we calculated many degree-based topological indices, such as the First Zagreb, First hyper-Zagreb, First and Second Gourava, Reciprocal Randic, First and Second K-Banhatti and Platt indices. These indices give significant numerical representations that summarise the structural attributes of the molecular network, providing insights into the compound's probable physicochemical properties.

Our findings underscore the relevance of topological indices in the analysis and characterisation of intricate molecular structures, especially for innovative 2D materials. The results endorse the extensive application of graph-theoretic models in cheminformatics and materials science, particularly for forecasting features pertinent to nanotechnology, spintronics and molecular electronics.

Future endeavors may encompass the expansion of this methodology to more categories of 2D frameworks and the investigation of relationships between calculated indices and empirically derived features, including magnetic anisotropy, bandgap and thermal stability. Moreover, machine learning algorithms utilizing topological indices might augment forecast accuracy in materials discovery and design.

References

[1] B. Huang, G. Clark, E. Navarro-Moratalla, D. R. Klein, R. Cheng, K. L. Seyler, D. Zhong, E. Schmidgall, M. A. McGuire, D. H. Cobden, W. Yao, D. Xiao, P. Jarillo-Herrero, and X. Xu, "Layer-dependent ferromagnetism in a van der Waals crystal down to the monolayer limit," *Nature*, vol. 546, no. 7657, pp. 270–273 (2017), doi: 10.1038/nature22391.

[2] Y. Deng, Y. Yu, Y. Song, J. Zhang, N. Z. Wang, Z. Sun, Y. Yi, Y. Wu, S. Wu, J. Zhu, J. Wang, X. H. Chen, and Y. Zhang, "Gate-tunable room-

temperature ferromagnetism in two-dimensional Fe_3GeTe_2," *Nature,* vol. 563, no. 7729, pp. 94–99 (2018), doi: 10.1038/s41586-018-0626-9.

[3] C. Felser, G. Fecher, and B. Balke, "Spintronics: A challenge for materials science and solid-state chemistry," *Angewandte Chemie International Edition*, vol. 46, no. 5, pp. 668–699 (2007), doi: 10.1002/anie.200601815.

[4] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A. Firsov, "Electric field effect in atomically thin carbon films," *Science*, vol. 306, no. 5696, pp. 666–669 (2004), doi: 10.1126/science.1102896.

[5] N. Papasimakis, S. Thongrattanasiri, N. I. Zheludev, and F. J. G. de Abajo, "The magnetic response of graphene split-ring metamaterials," *Light: Science & Applications*, vol. 2, no. 7, pp. 78–88 (2013), doi: 10.1038/lsa.2013.34.

[6] B. Radisavljevic, A. Radenovic, J. Brivio, V. Giacometti, and A. Kis, "Single-layer MoS_2 transistors," *Nature Nanotechnology,* vol. 6, no. 3, pp. 147–150 (2011), doi: 10.1038/nnano.2010.279.

[7] M. Corso, W. Auwärter, M. Muntwiler, A. Tamai, T. Greber, and J. Osterwalder, "Boron nitride nanomesh," *Science*, vol. 303, no. 5655, pp. 217–220 (2004), doi: 10.1126/science.1091979.

[8] M. R. Lukatskaya, O. Mashtalir, C. E. Ren, Y. Dall'Agnese, P. L. Taberna, P. Simon, M. W. Barsoum, and Y. Gogotsi, "Cation intercalation and high volumetric capacitance of two-dimensional titanium carbide," *Science,* vol. 341, no. 6153, pp. 1502–1505 (2013), doi: 10.1126/science.1241488.

[9] S. Y. Xie, X. B. Li, Y. Y. Sun, Y. L. Zhang, D. Han, W. Q. Tian, W. Q. Wang, Y. S. Zheng, S. B. Zhang, and H. B. Sun, "Theoretical characterization of reduction dynamics for graphene oxide by alkaline-earth metals," *Carbon*, vol. 52, pp. 122–127 (2012), doi: 10.1016/j.carbon.2012.09.012.

[10] P. Vogt, P. De Padova, C. Quaresima, J. Avila, E. Frantzeskakis, M. C. Asensio, A. Resta, B. Ealet, and G. Le Lay, "Silicene: compelling experimental evidence for graphenelike two-dimensional silicon," *Physical Review Letters*, vol. 108, no. 15, Art. no. 155501 (2012), doi: 10.1103/PhysRevLett.108.155501.

[11] S. Jungthawan, P. Reunchan, and S. Limpijumnong, "Theoretical study of strained porous graphene structures and their gas separa-

tion properties," *Carbon*, vol. 54, pp. 359–364 (2013), doi: 10.1016/j.carbon.2012.11.048.

[12] K. F. Mak, C. Lee, J. Hone, J. Shan, and T. F. Heinz, "Atomically thin MoS_2: A new direct-gap semiconductor," *Physical Review Letters*, vol. 105, no. 13, Art. no. 136805 (2010), doi: 10.1103/PhysRevLett.105.136805.

[13] C. Wu and M. Almuaalemi, "Synthesis of MOFs and characterization and drug loading efficiency," *ChemEngineering*, vol. 9, no. 2, Art. no. 24 (2025), doi: 10.3390/chemengineering9020024.

[14] F. Z. Zeggai, Z. Ait-Touchente, K. Bachari, and A. Elaissari, "Investigation of metal-organic frameworks (MOFs): Synthesis, properties and applications—An in-depth review," *Chemical Physics Impact*, Art. no. 100864 (2025), doi: 10.1016/j.chphi.2025.100864.

[15] M. S. Sardar and K. H. Hakami, "QSPR analysis of some Alzheimer's compounds via topological indices and regression models," *Journal of Chemistry*, vol. 2024, Art. no. 5520607 (2024), doi: 10.1155/2024/5520607.

[16] M. S. Sardar, M. A. Ali, F. Ashraf, and M. Cancan, "On topological indices of double and strong double graph of silicon carbide Si_2C_3-I[p,q]," *Journal of Medical and Pharmaceutical Chemistry Research*, vol. 5, pp. 37–49 (2023), doi: 10.22034/ecc.2023.356160.1519.

[17] M. S. Sardar, I. Siddique, F. Jarad, M. A. Ali, E. M. Türkan, and M. Danish, "Computation of vertex-based topological indices of middle graph of alkane (C_tH_{2t+2})," *Journal of Mathematics*, vol. 2022, Art. no. 8283898 (2022), doi: 10.1155/2022/8283898.

[18] P. Wang, X. Jiang, J. Hu, B. Wang, T. Zhou, H. Yuan, and J. Zhao, "Robust spin manipulation in 2D organometallic Kagome lattices: A first-principles study," *Physical Chemistry Chemical Physics*, vol. 22, no. 19, pp. 11045–11052 (2020), doi: 10.1039/D0CP00742K.

[19] X. Zhang, H. G. G. Reddy, A. Usha, M. C. Shanmukha, M. R. Farahani, and M. Alaeiyan, "A study on anti-malaria drugs using degree-based topological indices through QSPR analysis," *Mathematical Biosciences and Engineering*, vol. 20, no. 2, pp. 3594–3609 (2023), doi: 10.3934/mbe.2023167.

[20] D. Afzal, F. Afzal, M. R. Farahani, and S. Ali, "On computation of recently defined degree-based topological indices of some families of

convex polytopes via M-polynomial," *Complexity,* vol. 2021, Art. no. 5881476, pp. 1–11 (2021), doi: 10.1155/2021/5881476.

[21] F. Chaudhry, M. N. Husin, F. Afzal, D. Afzal, M. Ehsan, M. Cancan, and M. R. Farahani, "M-polynomials and degree-based topological indices of tadpole graph," *Journal of Discrete Mathematical Sciences and Cryptography,* vol. 24, no. 7, pp. 2059–2072 (2021), doi: 10.1080/09720529.2021.1984561.

[22] M. Azeem, A. Aslam, Z. Iqbal, M. A. Binyamin, and W. Gao, "Topological aspects of 2D structures of trans-Pd(NH_2)S lattice and a metal-organic superlattice," *Arabian Journal of Chemistry*, vol. 14, no. 3, Art. no. 102963 (2021), doi: 10.1016/j.arabjc.2020.102963.

[23] M. Alaeiyan, "Characteristics and eigenvalues of the newly defined Ala graph," *Physica Scripta*, vol. 100, no. 5, Art. no. 055201 (2025), doi: 10.1088/1402-4896/adc3d2.

Received June, 2025