

Computational analysis of some degree based topological indices of cubic structured tungsten trioxide [l,m,n] nanomultilayer

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Topological indices are numerical invariants of molecular graphs and are beneficial for predicting the physicochemical properties of chemical compounds. In this view, a topological index can be considered as a score function which maps each molecular structure to a real number. In the past two decades, tungsten trioxide (WO_3) nanostructures have been extensively studied for their diverse technological applications. They have received greater attention by researchers, owing to their novel functionalities and unique physicochemical properties. We, for the first time, compute the Sum Connectivity index, Variable Sum index, ABC index, Harmonic index, Ordinary Geometric Arithmetic index, SK indices, Forgotten index, Symmetric Division index, Augmented Zagreb index, Inverse sum index, IRM index, Modified second Zagreb index, Inverse Randić index, Albertson and Bell topological indices of cubic structured WO_3 [l, m, n] nanomultilayer. We also present a graphical analysis of all indices with respect to the dimension of this nanomultilayer.

Keywords: topological index, chemical graph, cubic WO_3 , nanomultilayer.

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1. Introduction

Let $G = (V, E)$ be a molecular graph of order p (number of vertices) with size q (number of edges). Denote uv , the link (edge) joining the nodes (vertices) u and v . The degree of a vertex $u \in V(G)$ is denoted by d_u and is the number of vertices that are adjacent to u . Molecular graphs are a unique type of chemical graphs, which describe the constitution of molecules [1]. Molecular graph considered in this article is finite, undirected, connected, loopless, and without multiple edges.

1.1. Background

Testing of new reagents in chemical physics and physical chemistry is always a major concern. One of the prominent strategies to address this issue is the graph theoretic approach, which performs to model the characteristics of novel and proposed chemical compounds to save time and costs. Chemical graph theory plays a crucial role in molecular topology and computational nanomaterials to determine the structure of molecular graphs [2–4]. Topological characterization is a standout approach provided by chemical graph theory to predict certain physicochemical properties like molecular weight, density, risk assessment, toxicity and determine regularity decisions and so forth [2–6]. Topological indices (molecular descriptors) are numerical values associated with chemical constitution and are applied in the development of quantitative structure-activity relationships (QSARs), Quantitative Structure Property Relationships (QSPRs) and Quantitative Structure-Toxicity Relationships (QSTRs) [7, 8]. They preserve the symmetry of molecular structures and act as a bridging tool between mathematics and chemistry. Until recently, several kinds of topological indices are introduced like distance-based, degree-based and spectrum-based indices and so on. Among them, degree based topological indices are robust in nature, because they can be directly derived from the structure of chemical graphs. The concept of topological indices in chemical graph theory was first introduced by Weiner in 1947, to predict the heats of formation, chromatographic retention time, boiling point and strain energy [2]. In recent times, many authors employed topological indices of various nanostructures involving Pent-Heptagonal Nanosheets [9], poly-hex nanotubes [10] and nanostar dendrimers [11]. For more about the significance of topological indices in molecular chemistry and the graph theoretical tools used in this article, we refer [12, 13] and references therein.

1.2. Degree based Topological Indices

In this part, we shall enumerate some degree-based topological indices (as explicated in Table 3) that will be needed in the main result section. Gutman et al. [3] established a pair of topological indices namely, first Zagreb ($M_1(G)$) and second Zagreb ($M_2(G)$) indices for predicting total π electron energy of compounds. In mathematical chemistry, there is a large number of topological indices of the form

$$TI = TI(G) = \sum_{x_i x_j \in E(G)} F(d_i, d_j).$$

Another important degree-based topological index called Randić index (connectivity index or branching index), which is given by Milan Randić in 1975 [32]. It has found manifold applications in drug designing field. Later, Amić et al. [29] proposed the generalized version of Inverse Randić index (for any real number α). For $\alpha = -1$, RR_α turns out to be a second Zagreb index; for $\alpha = 1$, RR_α will be a modified second Zagreb index and RR_α becomes a Reciprocal Randić index if $\alpha = -\frac{1}{2}$.

1.3. A brief sketch on WO_3 nanomaterial

Today has witnessed the prompt advancements in nanotechnology, which keeps in pace with the emergence of novel nanomaterials and interdisciplinary approaches. WO_3 is one such nanomaterial which has drawn considerable attention of research community due to their various applications in chemical sensors, field emission devices, electrochromic, photocatalysts [33] and photo-electrochemical water splitting [34]. For more details we refer [35] and references therein.

1.4. Proposed work and organization

Motivated by the formation of WO_3 nanomultilayer reported in [36], here, we construct a molecular graph for cubic WO_3 nanomultilayer and compute certain degree based topological indices to reveal its mathematical aspects. The partitions of the edge set and the vertex set of cubic WO_3 nanomultilayer have been well discussed in Section 2. In Section 3, we established our new results about cubic WO_3 nanomultilayer in terms of the parameters l , m and n . In order to disclose the trends of dependency among the values of indices and the dimensions of the nanomultilayer, some relevant graphical representations are provided in Section 4.

2. Methods

It is evident from Fig. 1 and Fig. 2 that, each tungsten atom is closely bound to six oxygen atoms, and each oxygen atom and two tungsten atoms are nearly adjacent, then each tungsten atom is a sub-neighbor with another one. As seen in Fig. 2(a), the intervening portion between two horizontal linear arrangements of connected tungsten trioxide molecules can be taken as a single row ($l = 1$). The same vertical alignment of this pattern forms a single column ($m = 1$) and these two parameters joined together to form a single layer ($n = 1$). Consider a 3-D cubic system of WO_3 nanomultilayer with l rows, m columns and n layers, and each layer contains l rows and m columns as shown in Fig. 3. Such a typical molecular system, atoms and bonds can be represented by vertices and edges, respectively. We reserve the notation $\text{c-WO}_3 [l, m, n]$ for cubic WO_3 nanomultilayer, where $l, m, n \geq 1$. The construction of $\text{c-WO}_3 [1, 1, 2]$ and $\text{c-WO}_3 [1, 3, 2]$ are illustrated in Fig. 2(b) and Fig. 2(c).

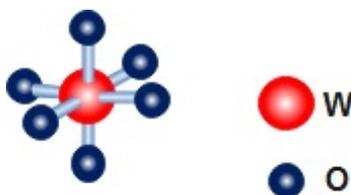


FIG. 1. A 3-D structure of WO_3 molecule

Observe that, $\text{c-WO}_3 [l, m, n]$ consist of 1,2 and 6 degrees vertices, and the total number of vertices are $4lmn + 6n + 15(ln + mn) + lm + l + m + 1$. Further, we partition the edge set of $\text{c-WO}_3 [l, m, n]$ into two disjoint sub-classes with respect to the degrees of the end vertices of each edge namely, $\{1,6\}$ and $\{2,6\}$, and the total number of edges are $6n(lm + l + m + 1)$. In other words, all surface O atoms bound to W atoms can be shown by the edge type $E_{(1,6)}$

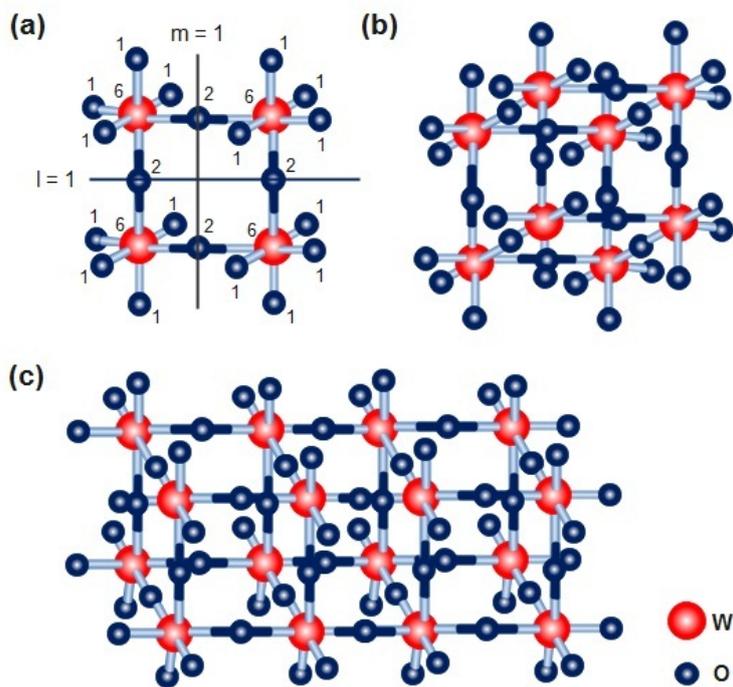


FIG. 2. (a) Vertices of $c\text{-WO}_3$ [1, 1, 1] labelled with degrees $\{1,2,6\}$; (b) $c\text{-WO}_3$ [1, 1, 2] and (c) $c\text{-WO}_3$ [1, 3, 2] nanomultilayer

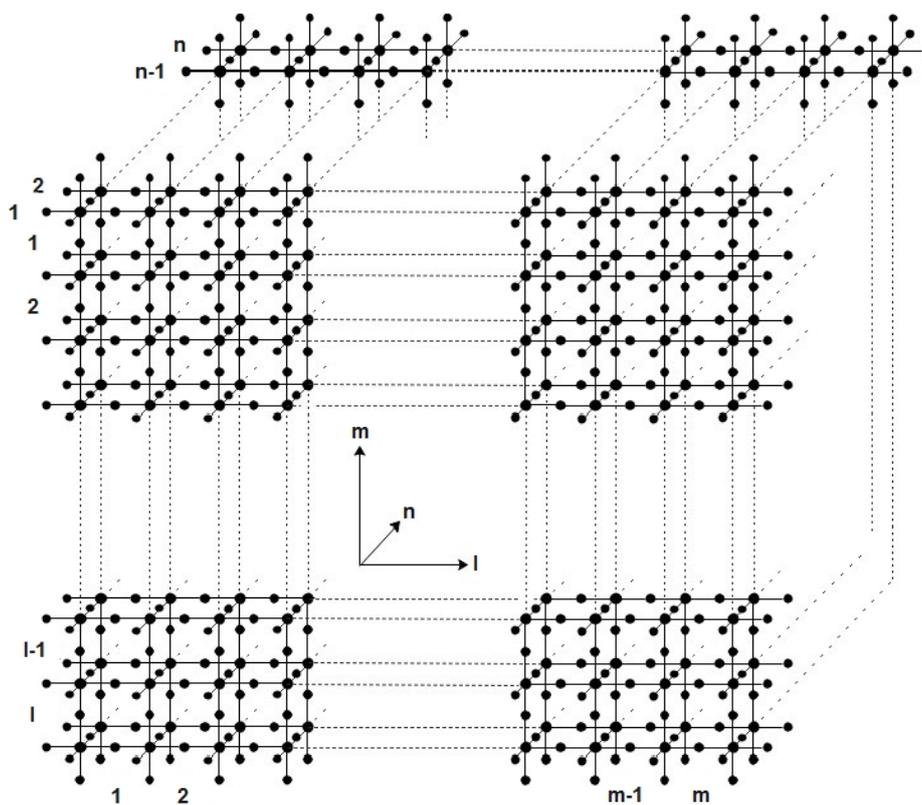


FIG. 3. Molecular graph of cubic -WO_3 [l, m, n] nanomultilayer

TABLE 1. Edge partition of c-WO₃ [l, m, n] nanomultilayer based on the degree of end vertices of each edge

Type of edges	$E_{(1, 6)}$	$E_{(2, 6)}$
$(d_u, d_v), u, v \in E(G)$	(1, 6)	(2, 6)
Number of Edges $ E_{(d_u, d_v)} $	$2(lm + mn + ln + l + m + 2n + 1)$	$6lmn + 4(ln + mn) + 2n - 2(lm + l + m + 1)$

TABLE 2. Vertex partition of c-WO₃ [l, m, n] nanomultilayer based on the degree of end vertices of each edge

Vertex partition V_{d_u}	V_1	V_2	V_6
$d_u, u \in V(G)$	1	2	6
Number of Vertices $ V_{d_u} $	$2(lm + mn + ln + l + m + 2n + 1)$	$3lmn + 2(ln + mn) - (lm + l + m + n + 1)$	$(lm + l + m + 1)n$

and the intermediated O atoms connected with W atoms are represented by the edge type $E_{(2, 6)}$. Table 1 and Table 2 represent the degree based edge partition and vertex partition of c-WO₃ [l, m, n].

The edge set c-WO₃ [l, m, n] nanomultilayer with $l, m, n \geq 1$ has following two partitions:

$$E_{(1, 6)} = \{e = uv \in E(c - \text{WO}_3 [l, m, n]) | d_u = 1, d_v = 6\}$$

and

$$E_{(2, 6)} = \{e = uv \in E(c - \text{WO}_3 [l, m, n]) | d_u = 2, d_v = 6\}.$$

The vertex set of c-WO₃ [l, m, n] nanomultilayer with $l, m, n \geq 1$ has following three partitions:

$$V_1 = \{v \in V(c - \text{WO}_3 [l, m, n]) | d_v = 1\}, \quad V_2 = \{v \in V(c - \text{WO}_3 [l, m, n]) | d_v = 2\}$$

and

$$V_6 = \{v \in V(c - \text{WO}_3 [l, m, n]) | d_v = 6\}.$$

3. Main results

Theorem 3.1. Let c-WO₃ [l, m, n] be the cubic structured WO₃ nanomultilayer of dimensions l, m, and $n \geq 1$. Then

(1)

$$\text{SCI}(c - \text{WO}_3 [l, m, n]) = \chi(c - \text{WO}_3 [l, m, n]) = \frac{2(lm + mn + nl + l + m + 2n + 1)}{\sqrt{7}} + \frac{6lmn + 4(ln + mn) + 2n - 2(lm + l + m + 1)}{2\sqrt{2}}.$$

(2)

$$\chi_\alpha(c - \text{WO}_3 [l, m, n]) = 2(lm + mn + nl + l + m + 2n + 1)(7)^\alpha + (6lmn + 4(ln + mn) + 2n - 2(lm + l + m + 1))(8)^\alpha.$$

(3)

$$\text{SEI}_\alpha(c - \text{WO}_3 [l, m, n]) = 2\alpha(lm + mn + nl + l + m + 2n + 1) + \alpha^2(3lmn + 2(ln + mn) - (lm + l + m + n + 1)) + \alpha^6(lm + l + m + 1)n,$$

where α is any positive real number such that $\alpha \neq 1$.

(4)

$$ABC(c - WO_3 [l, m, n]) = 2\sqrt{\frac{5}{6}}(lm + mn + nl + l + m + 2n + 1) + \sqrt{\frac{1}{2}}(6lmn + 4(ln + mn) + 2n - 2(lm + l + m + 1)).$$

(5)

$$H(c - WO_3 [l, m, n]) = \frac{4}{7}(lm + mn + nl + l + m + 2n + 1) + \frac{1}{4}(6lmn + 4(ln + mn) + 2n - 2(lm + l + m + 1)).$$

(6)

$$OGA(c - WO_3 [l, m, n]) = \frac{4\sqrt{6}}{7}(lm + mn + nl + l + m + 2n + 1) + \frac{\sqrt{3}}{2}(6lmn + 4(ln + mn) + 2n - 2(lm + l + m + 1)).$$

$$(7) SK(c - WO_3 [l, m, n]) = 24lmn + 23(ln + mn) + (22n - lm) - (l + m + 1).$$

$$(8) SK_1(c - WO_3 [l, m, n]) = 36lmn + 30(ln + mn) + 6(4n - lm) - 6(l + m + 1).$$

$$(9) SK_2(c - WO_3 [l, m, n]) = 96lmn + 88.5(ln + mn) + (81n - 7.5lm) - 7.5(l + m + 1).$$

$$(10) F(c - WO_3 [l, m, n]) = 240lmn + 234(ln + mn) + 6(38n - lm) - 6(l + m + 1).$$

$$(11) SDD(c - WO_3 [l, m, n]) = 20lmn + \frac{77}{3}(ln + mn) + \frac{1}{3}(94n + 17lm) + \frac{17}{3}(l + m + 1).$$

$$(12) AZI(c - WO_3 [l, m, n]) = 48lmn + 35.456(ln + mn) + (22.912n - 12.544lm) - 12.544(l + m + 1).$$

$$(13) ISI(c - WO_3 [l, m, n]) = 9lmn + 7.714(ln + mn) + 1.29(5n - lm) - 1.29(l + m + 1).$$

$$(14) IRM(c - WO_3 [l, m, n]) = 96lmn + 114(ln + mn) + (132n - 18lm) + 18(l + m + 1).$$

$$(15) {}^m M_2(c - WO_3 [l, m, n]) = \left(\frac{1}{6}\right)(3lmn + 4(ln + mn) + (5n + lm) + (l + m + 1)).$$

(16)

$$RR_\alpha(c - WO_3 [l, m, n]) = \frac{2}{(6)^\alpha}(lm + mn + nl + l + m + 2n + 1) + \frac{1}{(12)^\alpha}(6lmn + 4(ln + mn) + 2n - 2(lm + l + m + 1)).$$

$$(17) A(c - WO_3 [l, m, n]) = 24lmn + 26(ln + mn) + 2(14n + lm) + 2(l + m + 1).$$

(18)

$$B(c - WO_3 [l, m, n]) = 2(lm + mn + nl + l + m + 2n + 1) \left(1 - \frac{12n(lm + l + m + 1)}{4lmn + 6n + 15(ln + mn) + lm + l + m + 1}\right)^2 + (3lmn + 2(ln + mn) - (lm + l + m + n + 1)) \left(2 - \frac{12n(lm + l + m + 1)}{4lmn + 6n + 15(ln + mn) + lm + l + m + 1}\right)^2 + (lm + l + m + 1)n \left(6 - \frac{12n(lm + l + m + 1)}{4lmn + 6n + 15(ln + mn) + lm + l + m + 1}\right)^2.$$

Proof. One can make calculations in accordance with the rules presented in Table 3.

4. Index analysis and description

In this part, we present index analysis of computed indices of cubic $WO_3 [l, m, n]$ nanomultilayer. Fig. 4(a) suggests that IRM , Albertson and Bell indices are linearly related with number of vertices in nanomultilayer of dimensions l , m and n . These three indices really correlate the tendency of irregularity in structure [27, 30, 31]. However $B(G)$ progresses very slowly. On the other hand, $IRM(G)$ increases sharply, indicating that the nanomultilayer structure becomes more irregular and complex as dimension increases. The graph in Fig. 4(b) illustrates the dependence of $ABC(G)$, $OGA(G)$ and $AZI(G)$ on nanomultilayer dimension. It is now an established fact that, these indices are more sensitive to predict thermodynamic properties of compounds [18, 21, 25].

TABLE 3. Formula for degree-based topological indices of a graph G

S. No	Topological Index	Notation	Formula of Topological Index
1.	Sum Connectivity Index [14]	$SCI(G) = \chi(G)$	$\sum_{u,v \in E(G)} \frac{1}{\sqrt{d_u + d_v}}$
2.	General Sum Connectivity Index [15]	$\chi_\alpha(G)$	$\sum_{u,v \in E(G)} (d_u + d_v)^\alpha$
3.	Variable Sum exdeg Index [16, 17]	$SEI_\alpha(G)$	$\sum_{u \in V(G)} d_u(\alpha)^{d_u}$, and $\alpha \neq 1$
4.	Atomic Bond Connectivity Index [18]	$ABC(G)$	$\sum_{u,v \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u \cdot d_v}}$
5.	Harmonic Index [19, 20]	$H(G)$	$\sum_{u,v \in E(G)} \frac{2}{d_u + d_v}$
6.	Ordinary Geometric Arithmetic Index [21]	$OGA(G)$	$\sum_{u,v \in E(G)} \frac{2\sqrt{d_u \cdot d_v}}{d_u + d_v}$
7.	SK Index [22]	$SK(G)$	$\sum_{u,v \in E(G)} \frac{d_u + d_v}{2}$
8.	SK_1 Index [22]	$SK_1(G)$	$\sum_{u,v \in E(G)} \frac{d_u \cdot d_v}{2}$
9.	SK_2 Index [22]	$SK_2(G)$	$\sum_{u,v \in E(G)} \left(\frac{d_u + d_v}{2}\right)^2$
10.	Forgotten Index [23]	$F(G)$	$\sum_{u,v \in E(G)} [(d_u)^2 + (d_v)^2]$
11.	Symmetric Division (Deg) Index [24]	$SDD(G)$	$\sum_{u,v \in E(G)} \left[\frac{\min\{d_u, d_v\}}{\max\{d_u, d_v\}} + \frac{\max\{d_u, d_v\}}{\min\{d_u, d_v\}} \right]$
12.	Augmented Zagreb Index [25]	$AZI(G)$	$\sum_{u,v \in E(G)} \left(\frac{d_u \cdot d_v}{d_u + d_v - 2}\right)^3$
13.	Inverse sum (Indeg) Index [26]	$ISI(G)$	$\sum_{u,v \in E(G)} \frac{d_u \cdot d_v}{d_u + d_v}$
14.	IRM Index [27]	$IRM(G)$	$\sum_{u,v \in E(G)} (d_u - d_v)^2$
15.	Modified Second Zagreb Index [28]	${}^m M_2(G)$	$\sum_{u,v \in E(G)} \frac{1}{d_u \cdot d_v}$
16.	Inverse Randić Index [29]	$RR_\alpha(G)$	$\sum_{u,v \in E(G)} \frac{1}{(d_u \cdot d_v)^\alpha}$
17.	Albertson Index [30]	$A(G)$	$\sum_{u,v \in E(G)} d_u - d_v $
18.	Bell Index [31]	$B(G)$	$\sum_{u \in V(G)} \left(d_u - \frac{2q}{p}\right)^2$

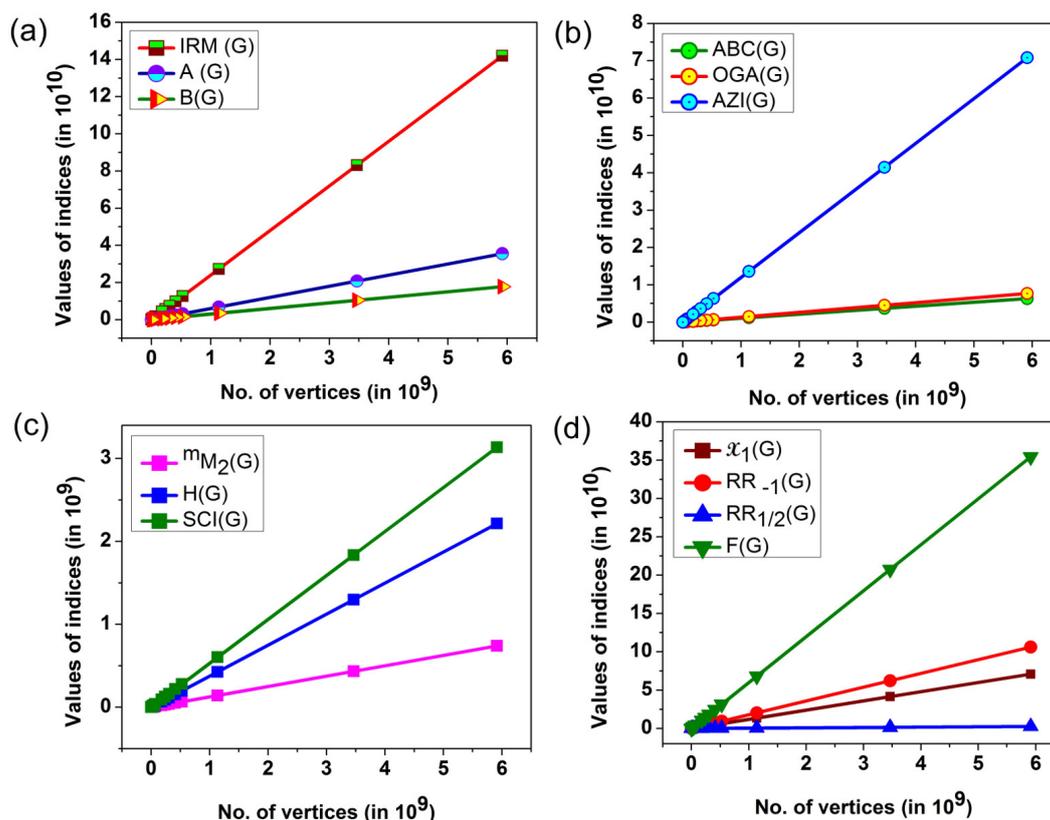


FIG. 4. Comparison of values of different topological indices (a) $IRM(G)$, $A(G)$ and $B(G)$; (b) $ABC(G)$, $OGA(G)$ and $AZI(G)$; (c) ${}^mM_2(G)$, $H(G)$ and $SCI(G)$ and (d) $\chi_1(G)$, $RR_{-1}(G)$, $RR_{1/2}(G)$ and $F(G)$ with respect to number of vertices in c-WO₃ [l, m, n] nanomultilayer

The indices graphically represented in Fig. 4(c) and Fig. 4(d) are actually related with the total π electron energy of compounds [14, 15, 19, 20, 28, 29]. Clearly, Forgotten index responds promptly as compared to other indices, suggesting that which has the higher prediction capacity of this energy. It is evident from Fig. 4(c) that, ${}^mM_2(G)$ has the least prediction potential with respect to the dimension. The indices plotted in Fig. 5(a) are considered to predict the total surface area of a structure [24, 26]. The prediction performance of $SDD(G)$ is greater than $ISI(G)$. Fig. 5(b) and Fig. 6 clearly show that, $SK_2(G)$ increases quickly as a function of dimensions [l, m, n].

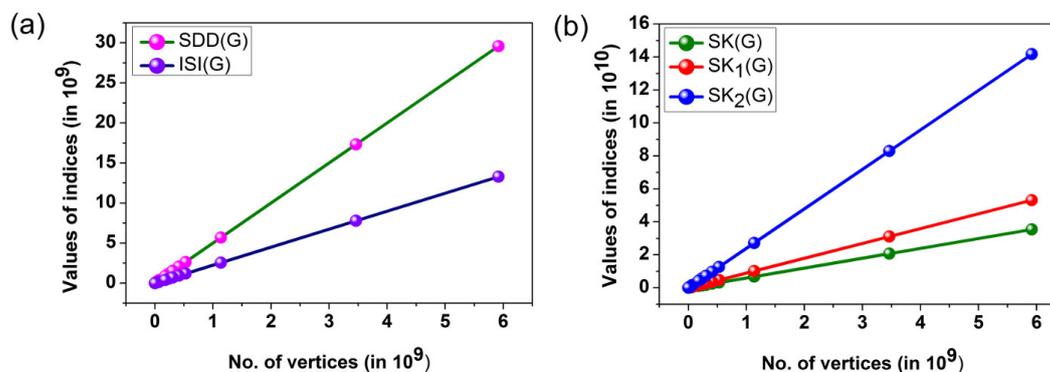


FIG. 5. Comparison of the topological indices (a) $SDD(G)$ and $ISI(G)$; (b) $SK(G)$, $SK_1(G)$ and $SK_2(G)$ with respect to number of vertices in c-WO₃ [l, m, n] nanomultilayer

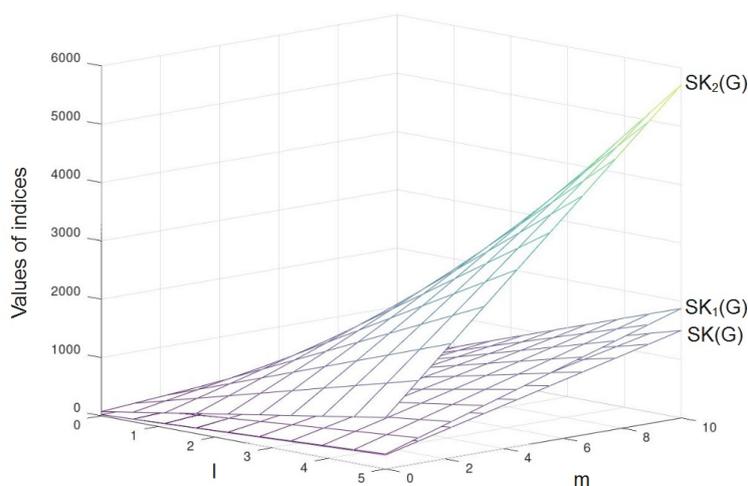


FIG. 6. A 3-D surface plot showing the comparison of $SK(G)$, $SK_1(G)$ and $SK_2(G)$ indices with respect to number of vertices in $c\text{-WO}_3 [l, m, n]$ monolayer; where $l \in [1, 5]$ and $m \in [1, 10]$ using Octave software

5. Conclusion

We successfully computed some important degree based topological indices for cubic structured $\text{WO}_3 [l, m, n]$ nanomultilayer and accurate expressions have been obtained. We also presented index analysis graphically with a view to understand the dependence on the involved parameters $[l, m, n]$. From an applicative point of view, the indices reported in this literature are really correlated with physicochemical properties of WO_3 nanomultilayer and will be helpful for people employed within nanotechnology industries.

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