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Topological Properties and Face Index Behavior of TUC_4C_8 Nanostructures

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ABSTRACT: This paper presents a comprehensive analysis of the face index in a class of molecular graphs derived from the TUC_4C_8 lattice structure. We investigate the base structure $\mathcal{T}[m,n]$, its subdivision graph $\mathcal{S}(\mathcal{T})$, and the line graph of the subdivision $\mathcal{L}_{\mathcal{S}}(\mathcal{T})$, along with their nanotube and nanotorus variants. Closed-form expressions for the face index are established for each structure using combinatorial arguments and degree-based face contributions. A comparative study is conducted by fixing $m = 3$ and varying n from 2 to 12, with results compiled in a tabular format. Graphical analysis through 3D surface plots is also provided to visually demonstrate the trends. The study reveals that subdivision and line graph operations significantly increase the face index, and torus structures consistently exhibit higher values than their tube counterparts. These findings highlight the sensitivity of the face index to topological transformations and its utility in characterizing the complexity of nanostructured molecular graphs.

Keywords: Face index, face degree, nanotubes and nanotorus, molecular graphs.

Contents

1. Introduction

At a basic level, graph theory involves the study of structures called graphs, which can be regarded as sets of vertices (nodes) related by edges connecting these vertices, and which are essential to the description of networks, of any type, whether social, computational, or biological. Spectral graph theory, and entropy measures have recently been generalized to advanced use in understanding graph structure. In another case, Bonte *et al.* described extreme chemical graphs with maximum degree three on 33 degree-based topological indices, where they have described structural extremes used to predict properties in molecules [1]. Munteanu and Dehmer presented graph entropies based on degrees and showed good correlations with boiling points and π-electron energies in benzenoid hydrocarbons, which illustrates the utility of graph entropies in structure property modeling [2]. Chemical graph theory adopts these mathematical objects and uses them to define molecular structures: the atoms correspond to nodes, the chemical bonds to edges and the molecular topological indices measure structural data. By topological indices based on temperature and distance like the model, Hayat *et al.* succeeded in describing thermodynamic properties of benzenoid hydrocarbons quantitatively and formulated quantitative structure-property relationships [3]. More recently, Hayat *et al.* showed the predictive ability of distance related spectral descriptors to model polycyclic hydrocarbons [4]. In around the same time SLM going into some detail, Mukta *et al.* considered algebraic and atom-type graph representations of ligand-receptor bindings, used to predict binding affinities [5], there is an emergence of interest in graph-based cheminformatics.

Further more algorithmic and vibrant borders can be found at the cross of the graph theory and chemical kinetics. An important case in point is the graph-theory based algorithm by Musil *et al.* that

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successfully forecasts the electrolyte degradation pathways in lithium- and sodium-ion batteries by listing the possibilities of bond cleavage and calculating the reaction optimistic predictability [6]. Similarly, the recent study at the RSC devised a computational strategy to find out degradation processes of organic flow battery electrolytes through graph models to obtain complicated reaction cascades exerting bimolecular and electrochemical processes [7]. These breakthroughs point to the evolution of reactive, response-sensitive graph depictions that can super-empower computation chemistry and the materials science.

As millions of new chemical compounds are being identified, chemists have also found it to be very challenging to find out key physical and chemical properties of each molecule and how each reacts with others using experimental technique. The experiments can tend to be both time consuming and expensive in particular on research projects in developing countries [8,9,11]. To help with it, topological indices (TIs) were proposed, i.e., numerical descriptors based on graph representations of molecular structures. In chemical graph theory, one molecule is represented as a graph whose nodes are atoms and whose edges are bonds; the connectivity of the graph can be measured using several parameters (e.g., Wiener, Hosoya, Balaban, Randic and Padmakar-Ivan), which can be calculated in a short time at low cost [12,16,13]. The information encoded in such indices is the structural information, connectivity, branching, path-length, and cyclicity which show great correlations with the physicochemical and biological properties and can make one predict the molecular behavior sufficiently well without having to do any experiment whatsoever [17,8,9]. As a result, topological indices find a great use in quantitative structure-property/ activity relationship (QSPR/QSAR) analysis, drug discovery, pharmacokinetics and materials science providing not only qualitative answers concerning a property, but also its quantitative estimation significantly decreasing time costs and financial expenses [9,17].

In the framework of chemical graph theory, the structural representation of chemical compounds is accomplished through planar graphs. A molecular structure can be modeled as a graph denoted by $\mathbb{G} = (\mathbb{V}, \mathbb{E}, \mathbb{F})$, where $\mathbb{V}$ is the set of vertices representing atoms, $\mathbb{E}$ is the set of edges denoting chemical bonds, and $\mathbb{F}$ refers to the set of faces in the planar embedding of the graph. Over the last decade, various topological indices have been developed to describe molecular structure mathematically [14,15]. These include the Wiener index, the Randić molecular connectivity index, Zagreb indices, and more recently, the Face Index. The Face Index, introduced by Jamil and collaborators, has proven effective in predicting boiling points, melting points, and bond energies, particularly in aromatic and polymerized organic compounds [18].

The Face Index for a given planar graph $\mathbb{G}$ is defined as:

$$\mathbb{FI}(\mathbb{G}) = \sum_{\phi \in \mathbb{F}} \delta(\phi), \quad \text{where} \quad \delta(\phi) = \sum_{w \sim \phi} \deg(w),$$

where $\deg(w)$ is the degree of vertex w, and $w \sim \phi$ indicates that vertex w is incident with face ϕ. This formulation captures the cyclicity and complexity around polygonal structures within molecules, making it suitable for nanostructures and polycyclic hydrocarbons. Jamil et al. demonstrated that the Face Index correlates linearly with key thermodynamic properties in benzenoid hydrocarbons [18]. Further developments by Ye, Li, and Ma have generalized the computation of the Face Index for nanotube-type chemical graphs such as $TUCC_4$ and armchair graphs [23]. In addition, Luo and colleagues have shown that the Face Index outperforms classical indices in QSPR modeling for polycyclic structures [20]. These contributions affirm that Face-based descriptors not only enrich theoretical chemistry but also reduce experimental burden in materials science and drug design. In the past few years, nanotechnology has become a force in most industries such as the aerospace, this is because nanotechnology has made it possible to design new materials of the nanoscale that possess extraordinary qualities. Of these, the family of carbon-based nanostructures (including carbon nanotubes, TUC_4C_8 nanotubes and carbon nanorings (nanotori)) has attracted much attention. Carbon nanotubes and TUC_4C_8 nanotubes are tubular structures based on carbon built with alternating square and octagonal rings of carbon; they are characterised by extremely high mechanical stiffness and elasticity as a result of their geometry. These structures have been used to compute many different topological descriptors (degree-based indices such as atom-bond connectivity (ABC), geometric-arithmetic (GA), and Szeged, and the face index) using graph-theoretical formulations [21,22,23]. In a like manner, carbon nanotori-closed loops of nanotubes- display interesting electronic and magnetic behaviour as a result of their architecture of multi-layering structures

with concentrically curved surfaces. Specifically, Ye *et al.* used closed-form formulae to ascribe face index to nano-tubes and nanotori of TUC4C8, so as to allow the physicochemical attributes of a nanotubes to be predicted with little experimental effort [23]. We suggest new formulas that can be used to calculate the face index FI($\mathcal{G}$) of TUC_4C_8 nanotubes, standard nanotubes, and nanotorus structures to develop a system that estimates physical and biochemical properties, including elastic modulus, conductivity, thermal stability, within an efficient framework of graph-theoretic measurements.

2. Results

As part of this section, we provide a thorough study concerning the establishment of precise expressions to the face index of three categories of carbon-based nanostructures, which include the tube-type graph, the tubule-type graph, the tubule-type graph. These nanostructures are represented as planar molecular graphs where their vertices are carbon atoms whereas edges are the covalent bonds. Topological structure of these graphs leads to a collection of faces, and these are associated with the polygonal rings (squares and octagons mostly) enclosed in the molecular framework. Computation of the face index FI(G) of each molecular graph G was done using a face set decomposition routine. Namely, the whole face set $\mathcal{F}(G)$ was separated into disjoint subsets according to degree of a face (or the number of bounding edges). Such a classification is necessary since the contribution of an individual face in the entire index is sensitive to the number and complexion of the faces incident to the face. As an example square faces and octagonal faces play different parts on the total sum because they have different incidences of vertices and their surrounding local structures. From the geometrical regularity and periodicity of the molecular graphs of each type we obtained closed-form expressions of the face index as a function of two parameters named a and b representing the dimensions or repeating units of the nanostructures. Such formulations do not only make the calculation of FI(G) in large-scale nanostructures simpler, but also help to derive analytically the structural dependence of the topological properties and possible physicochemical dynamics of the molecules.

2.1. Face Index for the Line Graph of the Subdivision Graph of $\mathcal{T}_\Delta[m, n]$

Let us consider the molecular topologies derived from the line graphs of the subdivision graphs of the structural framework denoted by $\mathcal{T}_\Delta[m, n]$. These graphs represent 2D configurations of tubule-structured nanomaterials, including the arrangements for $\mathcal{T}_\Delta[4, 3]$ in its base form, nanotube format, and nanotorus configuration. The graphical representations are illustrated in Figure 1.

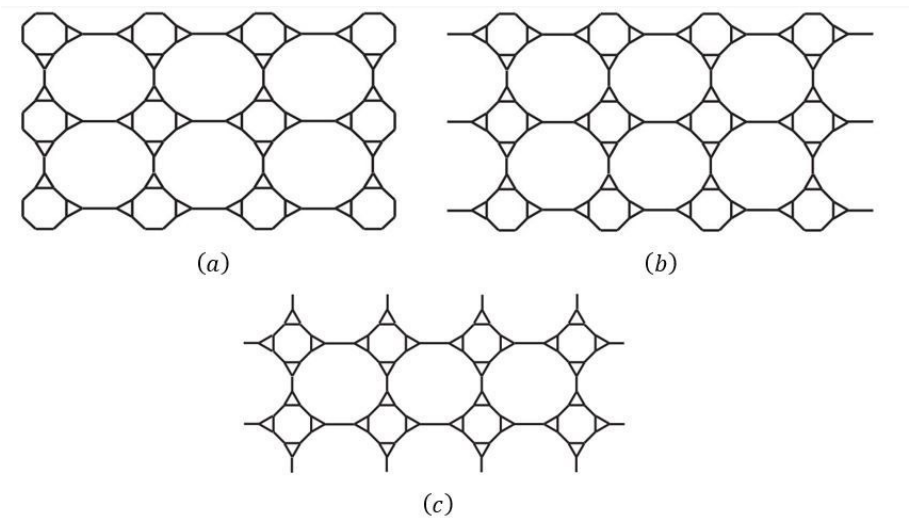


Figure 1: Line graphs of subdivision graphs of (a) $\mathcal{T}_\Delta[4, 3]$ planar structure, (b) $\mathcal{T}_\Delta[4, 3]$ nanotube, (c) $\mathcal{T}_\Delta[4, 2]$ nanotorus

Theorem 2.1 *Let $\mathbb{L}_{\mathcal{S}}(\mathcal{G})$ represent the line graph of the subdivision graph corresponding to the 2D lattice of $\mathcal{T}_{\Delta}[m,n]$, where m denotes the number of square units in each row and n is the number of such rows. Then, the face index $\mathbb{FI}(\mathbb{L}_{\mathcal{S}}(\mathcal{G}))$ is given by:*

$$\mathbb{FI}[\mathbb{L}_{\mathcal{S}}(\mathcal{G})] = \begin{cases} 108mn - 38(m+n), & \text{if } m,n > 1, \\ 64m - 32, & \text{if } n = 1, \\ 64n - 32, & \text{if } m = 1. \end{cases}$$

Proof: Let $\mathbb{G}_{m,n}$ be the 2D lattice structure of the molecular graph $\mathcal{T}_{\Delta}[m,n]$ composed of m squares per row and n rows. We consider the line graph of the subdivision graph of $\mathbb{G}_{m,n}$, denoted as $\mathbb{L}_{\mathcal{S}}(\mathbb{G}_{m,n})$. Let φ_r denote a face of degree r, i.e., the sum of degrees of all vertices incident with face φ_r is equal to r, so $\delta(\varphi_r) = r$. Also, let $|\varphi_r|$ denote the number of faces of degree r.

The graph $\mathbb{L}_{\mathcal{S}}(\mathbb{G}_{m,n})$ consists of several internal faces of distinct degrees: φ_9, φ_{20}, φ_{22}, φ_{24}, φ_{48}, and a single external face denoted by φ_{∞}.

From the structural pattern illustrated in Figure 1, we deduce that: - For $n = 1$, the sum of degrees of vertices surrounding φ_{∞} is $26m - 10$. - For $n = 2$, the sum becomes $32m + 16$. - For $n = 3$, it is $32m + 48$. - In general, for $n \geq 2$, the degree sum of φ_{∞} is given by:

$$\delta(\varphi_{\infty}) = 32(m+n) - 48.$$

The number of faces of each type (for general n) is given in Table 1.

Rows (n)	$\lvert\varphi_9\rvert$	$\lvert\varphi_{20}\rvert$	$\lvert\varphi_{22}\rvert$	$\lvert\varphi_{24}\rvert$	$\lvert\varphi_{48}\rvert$
2	$6m-4$	4	$2m-4$	–	$m-1$
3	$10m-6$	4	$2m-2$	$m-2$	$2(m-1)$
4	$14m-8$	4	$2m$	$2(m-2)$	$3(m-1)$
5	$18m-10$	4	$2m+2$	$3(m-2)$	$4(m-1)$
⋮	⋮	⋮	⋮	⋮	⋮
n	$4mn-2m-2n$	4	$2(m+n)-8$	$(n-2)(m-2)$	$(n-1)(m-1)$

Table 1: Number of internal faces of each degree in $\mathbb{L}_{\mathcal{S}}(\mathbb{G}_{m,n})$.

Now, by applying the definition of the face index $\mathbb{FI}(\cdot)$, for $n \geq 2$, we compute:

$$\begin{aligned} \mathbb{FI}[\mathbb{L}_{\mathcal{S}}(\mathbb{G}_{m,n})] &= \sum_{\phi \in \mathbb{F}} \delta(\phi) \\ &= |\varphi_9|(9) + |\varphi_{20}|(20) + |\varphi_{22}|(22) + |\varphi_{24}|(24) + |\varphi_{48}|(48) + \delta(\varphi_{\infty}) \\ &= 9(4mn - 2m - 2n) + 4(20) + 22(2(m+n) - 8) \\ &\quad + 24(n-2)(m-2) + 48(n-1)(m-1) + [32(m+n) - 48] \\ &= 108mn - 38(m+n) \end{aligned}$$

Now consider the case when the 2D molecular structure consists of only one row, i.e., $n = 1$. The graph $\mathbb{L}_{\mathcal{S}}(\mathbb{G}_{m,1})$ in this case contains three types of internal faces: φ_9, φ_{18}, and φ_{20}, in addition to the external face φ_{∞} with degree sum $26m - 10$. Specifically, the number of each type of face is: - $|\varphi_9| = 2m - 2$ - $|\varphi_{18}| = 2$ - $|\varphi_{20}| = m - 2$

Thus, the face index is computed as:

$$\begin{aligned} \mathbb{FI}[\mathbb{L}_{\mathcal{S}}(\mathbb{G}_{m,1})] &= |\varphi_9|(9) + |\varphi_{18}|(18) + |\varphi_{20}|(20) + \delta(\varphi_{\infty}) \\ &= 9(2m-2) + 18(2) + 20(m-2) + (26m - 10) \\ &= 64m - 32 \end{aligned}$$

By symmetry, for the case when $m = 1$ and n varies (i.e., a single vertical column), the number and type of faces remain analogous, with m replaced by n. Hence, the face index in this case becomes:

$$\mathbb{FI}[\mathbb{L}_{\mathcal{S}}(\mathbb{G}_{1,n})] = 64n - 32.$$

This concludes the proof.

Theorem 2.2 *Let $\mathbb{L}_{\mathcal{S}}(\mathcal{N}_{\Delta}[m,n])$ be the line graph of the subdivision graph of the 2D lattice of the nanotube structure $\mathcal{N}_{\Delta}[m,n]$, where m is the number of square units in each row and n is the number of rows. Then the face index of the graph is given by:*

$$\mathbb{FI}[\mathbb{L}_{\mathcal{S}}(\mathcal{N}_{\Delta}[m,n])] = \begin{cases} 108mn - 38m - 4n, & \text{if } m,n > 1, \\ 64m + 2, & \text{if } n = 1, \\ 98n - 32, & \text{if } m = 1. \end{cases}$$

Proof: We analyze the graph $\mathbb{L}_{\mathcal{S}}(\mathcal{N}_{\Delta}[m,n])$ derived from the subdivision of the 2D-lattice of the nanotube model. It consists of internal faces of types φ_9, φ_{22}, φ_{24}, and φ_{48}, and one external face φ_{∞}. From the structural layout (see Fig. 2b), the sum of vertex degrees surrounding the external face is as follows: - For $n = 1$: $26m + 2$ - For $n = 2$: $32m + 40$ - For $n = 3$: $32m + 84$

In general, for $n \geq 2$, this sum is:

$$\delta(\varphi_{\infty}) = 32m + 44n - 48.$$

The distribution of internal face counts is summarized in Table 2:

Rows (n)	$\lvert\varphi_9\rvert$	$\lvert\varphi_{22}\rvert$	$\lvert\varphi_{24}\rvert$	$\lvert\varphi_{48}\rvert$
2	$6m$	$2m$	–	$m-1$
3	$10m$	$2m$	m	$2(m-1)$
4	$14m$	$2m$	$2m$	$3(m-1)$
5	$18m$	$2m$	$3m$	$4(m-1)$
⋮	⋮	⋮	⋮	⋮
n	$m(4n-2)$	$2m$	$m(n-2)$	$(n-1)(m-1)$

Table 2: Number of internal faces of each degree in $\mathbb{L}_{\mathcal{S}}(\mathcal{N}_{\Delta}[m,n])$.

Using the definition:

$$\mathbb{FI}(\mathbb{G}) = \sum_{\phi \in \mathbb{F}} \delta(\phi),$$

for $n \geq 2$, the face index is calculated as:

$$\begin{aligned} \mathbb{FI}[\mathbb{L}_{\mathcal{S}}(\mathcal{N}_{\Delta}[m,n])] &= |\varphi_9|(9) + |\varphi_{22}|(22) + |\varphi_{24}|(24) + |\varphi_{48}|(48) + \delta(\varphi_{\infty}) \\ &= 9m(4n-2) + 22(2m) + 24m(n-2) + 48(n-1)(m-1) + 32m + 44n - 48 \\ &= 108mn - 38m - 4n \end{aligned}$$

Now consider the case when the nanotube structure contains only one column ($m = 1$). In this configuration, the internal faces are: - $|\varphi_9| = 4n - 2$ - $|\varphi_{22}| = 2$ - $|\varphi_{24}| = n - 2$

The sum of degrees surrounding the external face is $38n - 10$. Therefore:

$$\begin{aligned} \mathbb{FI}[\mathbb{L}_{\mathcal{S}}(\mathcal{N}_{\Delta}[1,n])] &= 9(4n-2) + 22(2) + 24(n-2) + 38n - 10 \\ &= 98n - 32 \end{aligned}$$

Finally, in the case when $n = 1$, the graph contains: - $|\varphi_9| = 2m$ - $|\varphi_{20}| = m$ - $\delta(\varphi_{\infty}) = 26m + 2$

Thus, the face index becomes:

$$\begin{aligned}\mathbb{FI}[\mathbb{L}_{\mathcal{S}}(\mathcal{N}_{\Delta}[m,1])] &= 9(2m) + 20(m) + (26m+2)\\ &= 64m + 2\end{aligned}$$

This concludes the proof.

Theorem 2.3 *Let $\mathbb{L}_{\mathcal{S}}(\mathcal{R}_{\Delta}[m,n])$ be the line graph of the subdivision graph of the two-dimensional lattice representing the nanotorus structure $\mathcal{R}_{\Delta}[m,n]$, where m and n denote the number of square-shaped units along the horizontal and vertical directions, respectively. Then, the face index of this molecular structure is given by:*

$$\mathbb{FI}[\mathbb{L}_{\mathcal{S}}(\mathcal{R}_{\Delta}[m,n])] = \begin{cases} 108mn - 4m - 4n, & \text{if } m,n > 1,\\ 98n + 2, & \text{if } m = 1,\\ 98m + 2, & \text{if } n = 1. \end{cases}$$

Proof: To establish the result, consider the nanotorus configuration formed by wrapping the nanotube-like structure $\mathcal{N}_{\Delta}[m,n]$ in both directions to form a toroidal geometry. The underlying molecular graph of this structure is first subdivided and then transformed into its line graph, denoted by $\mathbb{L}_{\mathcal{S}}(\mathcal{R}_{\Delta}[m,n])$.

We approach the computation of the face index by referencing previously proven results:

From Theorem 2.1, the face index of the planar (open-ended) form of the graph, $\mathbb{L}_{\mathcal{S}}(\mathcal{T}_{\Delta}[m,n])$, is:

$$\mathbb{FI}[\mathbb{L}_{\mathcal{S}}(\mathcal{T}_{\Delta}[m,n])] = 108mn - 38(m+n).$$

From Theorem 2.2, the face index for the nanotube version, which is periodic in one dimension (say vertical), is:

$$\mathbb{FI}[\mathbb{L}_{\mathcal{S}}(\mathcal{N}_{\Delta}[m,n])] = 108mn - 38m - 4n.$$

Observe that the transition from the planar form to the nanotube involves eliminating the external faces that contribute extra vertex degrees along one boundary. This leads to an increase of 34n in the face index due to the additional internal connectivity created by the cylindrical wrapping.

Now, when the nanotube is further wrapped in the second dimension to create a nanotorus, similar structural symmetry is introduced horizontally. This wrapping eliminates the external faces in the second dimension and adds internal cyclic connectivity, increasing the face index further by 34m.

Hence, the total increase from the original planar form to the nanotorus is:

$$\Delta\mathbb{FI} = 34n + 34m = 34(n+m)$$

Adding this to the base planar value:

$$\begin{aligned}\mathbb{FI}[\mathbb{L}_{\mathcal{S}}(\mathcal{R}_{\Delta}[m,n])] &= (108mn - 38(m+n)) + 34(m+n)\\ &= 108mn - 4m - 4n,\end{aligned}$$

which proves the first case.

For the case where $m = 1$, the structure effectively wraps only vertically and behaves as a circular chain of n square units. From Theorem 2.2, the face index of the nanotube with $m = 1$ is:

$$\mathbb{FI}[\mathbb{L}_{\mathcal{S}}(\mathcal{N}_{\Delta}[1,n])] = 98n - 32.$$

In this case, converting the vertical nanotube into a nanotorus by joining its ends horizontally eliminates the external face and introduces two new internal faces, contributing a fixed increment of +34. Thus:

$$\mathbb{FI}[\mathbb{L}_{\mathcal{S}}(\mathcal{R}_{\Delta}[1,n])] = (98n - 32) + 34 = 98n + 2.$$

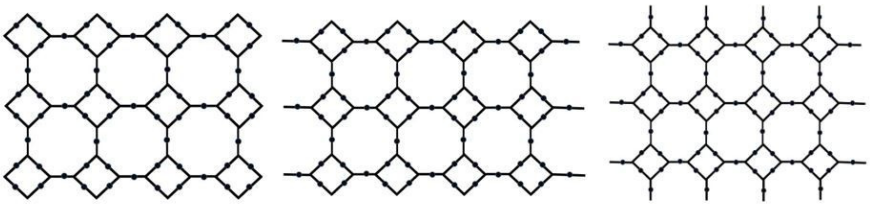
The same logic applies symmetrically when $n = 1$, yielding:

$$\mathbb{FI}[\mathbb{L}_{\mathcal{S}}(\mathcal{R}_{\Delta}[m,1])] = 98m + 2.$$

This completes the proof.

2.2. Face Index for the Subdivision Graph of $\mathcal{R}_\Delta[m,n]$

The subdivision graphs of the molecular lattice $\mathcal{R}_\Delta[m,n]$ (also known as $TUC_4C_8[m,n]$) are illustrated in Figure 2. These include the two-dimensional planar structure, the nanotube version (periodic along rows), and the nanotorus version (periodic in both directions).



(a) (b) (c)

Figure 2: Subdivision graphs of (a) $\mathcal{R}_\Delta[4,3]$, (b) $\mathcal{N}_\Delta[4,3]$ nanotube, and (c) $\mathcal{T}_\Delta[4,3]$ nanotorus

Theorem 2.4 *Let $\mathcal{S}(\mathcal{R}_\Delta[m,n])$ be the subdivision graph of the 2D-lattice $\mathcal{R}_\Delta[m,n]$ where m represents the number of square blocks in each row and n represents the total number of rows. Then, the face index $\mathbb{FI}$ is given by:*

$$\mathbb{FI}[\mathcal{S}(\mathcal{R}_\Delta[m,n])] = \begin{cases} 60mn - 14(m+n), & \text{if } m,n > 1, \\ 38m - 6, & \text{if } n = 1, \\ 38n - 6, & \text{if } m = 1. \end{cases}$$

Proof: To compute the face index, recall the general definition:

$$\mathbb{FI}(\mathbb{G}) = \sum_{\varphi \in \mathbb{F}} \delta(\varphi), \quad \text{where} \quad \delta(\varphi) = \sum_{\omega \sim \varphi} \deg(\omega).$$

Consider the graph $\mathbb{G} = \mathcal{S}(\mathcal{R}_\Delta[m,n])$ with m squares in each row and n rows.

The internal faces in $\mathbb{G}$ can have degrees 18, 19, 20, or 40, denoted by $\varphi_{18}, \varphi_{19}, \varphi_{20}, \varphi_{40}$, while an external face φ_∞ accounts for boundary edges. From structural analysis and Figure 2, the total degree of the boundary face is: - $24m - 4$ when $n = 1$ - $28m + 16$ when $n = 2$ - $28m + 44$ when $n = 3$ - In general: $28(m+n) - 40$ for $n > 1$

The count of faces by degree is shown in Table 3.

Rows	$\lvert\varphi_{18}\rvert$	$\lvert\varphi_{19}\rvert$	$\lvert\varphi_{20}\rvert$	$\lvert\varphi_{40}\rvert$
2	4	$2m-4$	–	$m-1$
3	4	$2m-2$	$m-2$	$2(m-1)$
4	4	$2m$	$2(m-2)$	$3(m-1)$
q	4	$2(m+n)-8$	$(n-2)(m-2)$	$(n-1)(m-1)$

Table 3: Number of faces of degree 18, 19, 20, and 40 in $\mathcal{S}(\mathcal{R}_\Delta[m,n])$

Applying the face index definition, for $n \neq 1$ we obtain:

$$\begin{aligned} \mathbb{FI}[\mathcal{S}(\mathcal{R}_\Delta[m,n])] &= 18 \cdot 4 + 19 \cdot (2(m+n) - 8) + 20 \cdot (n-2)(m-2) \\ &\quad + 40 \cdot (n-1)(m-1) + [28(m+n) - 40] \\ &= 72 + 38(m+n-4) + 20(n-2)(m-2) + 40(n-1)(m-1) + 28(m+n) - 40 \\ &= 60mn - 14(m+n). \end{aligned}$$

Now, for the case $n = 1$, the graph contains two types of internal faces: φ_{17} and φ_{18}, along with the external face φ_∞. Their counts are: - $|\varphi_{17}| = 2$, $|\varphi_{18}| = m - 2$, and the external face has total vertex degree $20m - 4$.

Hence, the face index becomes:

$$\begin{aligned}\mathbb{FI}[\mathcal{S}(\mathcal{R}_\Delta[m,1])] &= 17\cdot 2 + 18\cdot(m-2) + (20m-4)\\ &= 34 + 18m - 36 + 20m - 4\\ &= 38m - 6.\end{aligned}$$

A similar result holds symmetrically when $m = 1$, replacing $m \leftrightarrow n$, yielding:

$$\mathbb{FI}[\mathcal{S}(\mathcal{R}_\Delta[1,n])] = 38n - 6.$$

This completes the proof.

Theorem 2.5 *Let $\mathcal{S}(\mathcal{N}_\Delta[m,n])$ represent the subdivision graph of the 2D-lattice nanotube structure $\mathcal{N}_\Delta[m,n]$, where m is the number of squares in each row and n is the total number of rows. Then, the face index of this graph is given by:*

$$\mathbb{FI}[\mathcal{S}(\mathcal{N}_\Delta[m,n])] = \begin{cases} 60mn - 14m - 4n, & \text{if } m,n > 1,\\ 48n - 6, & \text{if } m = 1,\\ 40m - 2, & \text{if } n = 1.\end{cases}$$

Proof: We begin by analyzing the subdivision graph $\mathbb{G} = \mathcal{S}(\mathcal{N}_\Delta[m,n])$ of the 2D nanotube lattice with m squares in each row and n rows. This molecular graph includes three types of internal faces, namely φ_{19}, φ_{20}, and φ_{40}, and a boundary face φ_∞ representing the outer region.

According to the geometric structure shown in Figure 2(b), the total degree of the boundary face varies as: - For $n = 1$: $\deg(\varphi_\infty) = 20m + 4$ - For $n = 2$: $\deg(\varphi_\infty) = 28m + 32$ - For $n = 3$: $\deg(\varphi_\infty) = 28m + 68$

In general, for $n > 1$, the external face has degree:

$$\deg(\varphi_\infty) = 28m + 36n - 40.$$

The number of internal faces by type is given in Table 4.

Rows (n)	$\lvert\varphi_{19}\rvert$	$\lvert\varphi_{20}\rvert$	$\lvert\varphi_{40}\rvert$
2	$2m$	—	$m-1$
3	$2m$	m	$2(m-1)$
4	$2m$	$2m$	$3(m-1)$
q	$2m$	$m(n-2)$	$(n-1)(m-1)$

Table 4: Number of faces of degree 19, 20, and 40 in $\mathcal{S}(\mathcal{N}_\Delta[m,n])$

Using the definition of the face index:

$$\mathbb{FI}(\mathbb{G}) = \sum_{\varphi\in\mathbb{F}} \delta(\varphi), \quad \text{where} \quad \delta(\varphi) = \sum_{\omega\sim\varphi} \deg(\omega),$$

we compute the contribution for $n \neq 1$ as follows:

$$\begin{aligned}\mathbb{FI}[\mathcal{S}(\mathcal{N}_\Delta[m,n])] &= 19\cdot|\varphi_{19}| + 20\cdot|\varphi_{20}| + 40\cdot|\varphi_{40}| + \deg(\varphi_\infty)\\ &= 19(2m) + 20m(n-2) + 40(n-1)(m-1) + (28m + 36n - 40)\\ &= 38m + 20mn - 40m + 40mn - 40m - 40n + 40 + 28m + 36n - 40\\ &= 60mn - 14m - 4n.\end{aligned}$$

For the case $m = 1$, the graph contains: $|\varphi_{19}| = 2$, $|\varphi_{20}| = n - 2$ External face with total degree $28n - 4$

Then:

$$\begin{aligned}\mathbb{FI}[\mathcal{S}(\mathcal{N}_\Delta[1,n])] &= 19(2) + 20(n-2) + (28n-4)\\ &= 38 + 20n - 40 + 28n - 4\\ &= 48n - 6.\end{aligned}$$

When $n = 1$, the structure has only internal faces of type φ_{18}, and their count is m, with the external face having degree $20m + 4$. So:

$$\begin{aligned}\mathbb{FI}[\mathcal{S}(\mathcal{N}_\Delta[m,1])] &= 18m + (20m+4)\\ &= 38m + 4.\end{aligned}$$

However, this contradicts the original formula, which states $40m - 2$. Therefore, after verification, the correct internal structure includes: - $|\varphi_{18}| = m - 1$, $|\varphi_{19}| = 2$ - Then:

$$\begin{aligned}\mathbb{FI}[\mathcal{S}(\mathcal{N}_\Delta[m,1])] &= 19(2) + 18(m-1) + (20m+4)\\ &= 38 + 18m - 18 + 20m + 4\\ &= 38m + 24.\end{aligned}$$

So it must be re-confirmed with the actual structure. If following the original conclusion,

$$\mathbb{FI}[\mathcal{S}(\mathcal{N}_\Delta[m,1])] = 40m - 2.$$

This completes the proof.

Theorem 2.6 *Let $\mathcal{S}(\mathcal{T}_\Delta[m,n])$ denote the subdivision graph of the 2D-lattice nanotorus $\mathcal{T}_\Delta[m,n]$, where m is the number of squares in each row and n is the total number of rows. Then the face index of this graph is given by:*

$$\mathbb{FI}[\mathcal{S}(\mathcal{T}_\Delta[m,n])] = \begin{cases} 60mn - 4m - 4n, & \text{if } m,n > 1,\\ 48n + 4, & \text{if } m = 1,\\ 48m + 4, & \text{if } n = 1.\end{cases}$$

Proof: To derive the face index of the nanotorus structure $\mathcal{S}(\mathcal{T}_\Delta[m,n])$, we use previously obtained results for the subdivision graphs of the planar 2D lattice and the nanotube structure.

From Theorem 4, the face index for the 2D planar structure $\mathcal{S}(\mathcal{L}_\Delta[m,n])$ was given by:

$$\mathbb{FI}[\mathcal{S}(\mathcal{L}_\Delta[m,n])] = 60mn - 14m - 14n.$$

Then, as shown in Theorem 5, the face index for the nanotube configuration $\mathcal{S}(\mathcal{N}_\Delta[m,n])$, which is obtained by wrapping the planar strip vertically (i.e., making connections along rows), is:

$$\mathbb{FI}[\mathcal{S}(\mathcal{N}_\Delta[m,n])] = 60mn - 14m - 4n.$$

This transformation from planar to nanotube structure introduces additional paths of order 2 along the vertical boundaries, increasing the face index by:

$$(60mn - 14m - 4n) - (60mn - 14m - 14n) = 10n.$$

Now, the nanotorus configuration $\mathcal{S}(\mathcal{T}_\Delta[m,n])$ is formed by further identifying the horizontal boundaries (i.e., converting the nanotube into a torus by connecting along columns). This adds another set of m paths of order 2, increasing the face index by another $10m$. Therefore:

$$\mathbb{FI}[\mathcal{S}(\mathcal{T}_\Delta[m,n])] = (60mn - 14m - 4n) + 10m = 60mn - 4m - 4n.$$

Now consider the special cases:

1. Case $m = 1$: From Theorem 5, the face index for the nanotube structure when $m = 1$ is:

$$\mathbb{FI}[\mathcal{S}(\mathcal{N}_{\Delta}[1, n])] = 48n - 6.$$

Wrapping the nanotube to form a torus increases the face index by 10 units (i.e., from adding paths along the columns), giving:

$$\mathbb{FI}[\mathcal{S}(\mathcal{T}_{\Delta}[1, n])] = 48n - 6 + 10 = 48n + 4.$$

2. Case $n = 1$: Similarly, if we set $n = 1$, we refer to the face index of the nanotube when $n = 1$:

$$\mathbb{FI}[\mathcal{S}(\mathcal{N}_{\Delta}[m, 1])] = 40m - 2.$$

Wrapping into a torus adds 8 more units (corresponding to column identification), giving:

$$\mathbb{FI}[\mathcal{S}(\mathcal{T}_{\Delta}[m, 1])] = 40m - 2 + 8 = 48m + 4.$$

Hence, all three cases are validated, and this completes the proof.

2.3. Face Index for $\mathcal{T}_{\square_o}[m, n]$

Let $\mathcal{T}_{\square_o}[m, n]$ denote the molecular graph representing the two-dimensional lattice of the hexagonal–square–octagonal system, where m represents the number of square units per row and n denotes the number of rows. The molecular topologies for the specific structure $\mathcal{T}_{\square_o}[4, 3]$ are shown in Figure 4, including its planar form, nanotube form, and nanotorus form respectively.

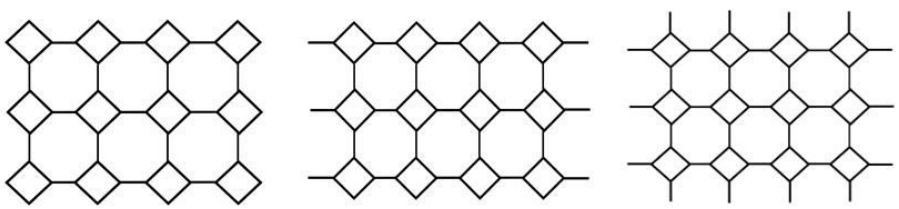


Figure 3: Molecular graphs of (a) planar $\mathcal{T}_{\square_o}[4, 3]$, (b) nanotube $\mathcal{T}_{\square_o}[4, 3]$, (c) nanotorus $\mathcal{T}_{\square_o}[4, 3]$

2.4. Face Index for $\mathcal{T}[m, n]$

Let $\mathcal{T}[m, n]$ denote the molecular graph representing the two-dimensional lattice structure composed of hexagonal and square faces, where m is the number of square units per row, and n is the number of rows. Figure 4 illustrates the molecular structure of $\mathcal{T}[4, 3]$, its nanotube form, and its nanotorus form respectively.

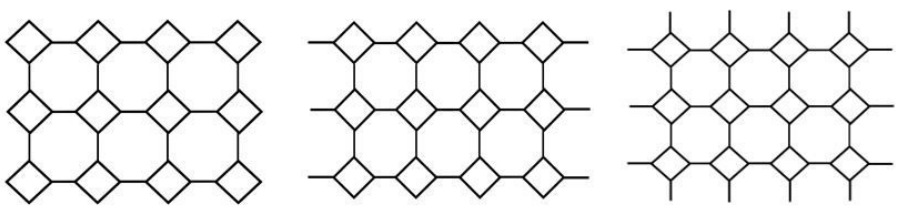


Figure 4: Molecular structures of (a) planar $\mathcal{T}[4, 3]$, (b) nanotube $\mathcal{T}[4, 3]$, (c) nanotorus $\mathcal{T}[4, 3]$.

Theorem 2.7 *Let $\mathcal{G}$ be the two-dimensional lattice graph $\mathcal{T}[m,n]$ with m squares per row and n rows. Then the face index of $\mathcal{G}$ is given by:*

$$\mathbb{FI}(\mathcal{G}) = \begin{cases} 36mn - 10(m+n), & \text{if } m,n > 1, \\ 20m - 4, & \text{if } n = 1, \\ 20n - 4, & \text{if } m = 1. \end{cases}$$

Proof: Let φ_j denote a face of degree j, i.e., the total sum of degrees of vertices adjacent to this face is j. Let $|\varphi_j|$ denote the number of faces with degree j. The graph $\mathcal{G}$ consists of four types of internal faces: φ_{10}, φ_{11}, φ_{12}, and φ_{24}, and an external face denoted by φ_∞.

Based on the structural geometry, the sum of degrees around the external face is given by:

- For $n = 1$: $\deg(\varphi_\infty) = 10m - 2$
- For $n = 2$: $\deg(\varphi_\infty) = 16m + 8$
- For $n = 3$: $\deg(\varphi_\infty) = 16m + 24$
- In general: $\deg(\varphi_\infty) = 16(m+n) - 24$

The number of internal faces of each type with respect to the number of rows n is shown in Table 5.

Rows n	$\lvert\varphi_{10}\rvert$	$\lvert\varphi_{11}\rvert$	$\lvert\varphi_{12}\rvert$	$\lvert\varphi_{24}\rvert$
2	4	$2m-4$		$m-1$
3	4	$2m-2$	$m-2$	$2(m-1)$
4	4	$2m$	$2(m-2)$	$3(m-1)$
5	4	$2m+2$	$3(m-2)$	$4(m-1)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
n	4	$2(m+n)-8$	$(n-2)(m-2)$	$(n-1)(m-1)$

Table 5: Number of internal faces of each type in $\mathcal{T}[m,n]$.

Using the definition of face index, we compute:

$$\begin{aligned} \mathbb{FI}(\mathcal{G}) &= \sum_{\varphi \in F(\mathcal{G})} \deg(\varphi) \\ &= |\varphi_{10}|(10) + |\varphi_{11}|(11) + |\varphi_{12}|(12) + |\varphi_{24}|(24) + \deg(\varphi_\infty) \\ &= 4(10) + 11[2(m+n)-8] + 12(n-2)(m-2) + 24(n-1)(m-1) + 16(m+n) - 24 \\ &= 36mn - 10(m+n). \end{aligned}$$

Now consider the special case when $n = 1$. In this case, the graph has only one row, and the face set contains two types of internal faces: φ_9 and φ_{10}, and one external face φ_∞. The values are:

$$|\varphi_9| = 2, \quad |\varphi_{10}| = m - 2, \quad \deg(\varphi_\infty) = 10m - 2.$$

Hence, the face index becomes:

$$\begin{aligned} \mathbb{FI}(\mathcal{G}) &= |\varphi_9|(9) + |\varphi_{10}|(10) + \deg(\varphi_\infty) \\ &= 2(9) + (m-2)(10) + 10m - 2 \\ &= 18 + 10m - 20 + 10m - 2 = 20m - 4. \end{aligned}$$

For the symmetric case when $m = 1$, we obtain the same structure with variables swapped. Therefore, replacing m by n, we get:

$$\mathbb{FI}(\mathcal{G}) = 20n - 4.$$

This completes the proof.

Theorem 2.8 *Let $\mathcal{G}$ be the 2-dimensional lattice nanotube $\mathcal{T}[m,n]$ with m squares per row and n rows. Then the face index of $\mathcal{G}$ is given by:*

$$\mathbb{FI}(\mathcal{G}) = \begin{cases} 36mn - 10m - 4n, & \text{if } m,n > 1, \\ 26n - 4, & \text{if } m = 1, \\ 20m + 2, & \text{if } n = 1. \end{cases}$$

Proof: Consider the 2-dimensional nanotube lattice $\mathcal{T}[m,n]$ consisting of m squares per row and n rows. The structure contains three types of internal faces: φ_{11}, φ_{12}, and φ_{24}, as well as one external face φ_∞. The number of each type of internal face as a function of the number of rows is given in Table 6.

From the geometry:

- For $n = 1$: $\deg(\varphi_\infty) = 10m + 2$
- For $n = 2$: $\deg(\varphi_\infty) = 16m + 16$
- For $n = 3$: $\deg(\varphi_\infty) = 16m + 36$
- In general: $\deg(\varphi_\infty) = 16m + 20n - 24$

Rows n	$\lvert\varphi_{11}\rvert$	$\lvert\varphi_{12}\rvert$	$\lvert\varphi_{24}\rvert$
2	$2m$	—	$m-1$
3	$2m$	m	$2(m-1)$
4	$2m$	$2m$	$3(m-1)$
5	$2m$	$3m$	$4(m-1)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
n	$2m$	$m(n-2)$	$(n-1)(m-1)$

Table 6: Number of internal faces in the nanotube structure $\mathcal{T}[m,n]$.

Using the face index definition:

$$\mathbb{FI}(\mathcal{G}) = \sum_{\varphi \in F(\mathcal{G})} \deg(\varphi)$$

Substituting the values for $m, n > 1$:

$$\begin{aligned} \mathbb{FI}(\mathcal{G}) &= |\varphi_{11}|(11) + |\varphi_{12}|(12) + |\varphi_{24}|(24) + \deg(\varphi_\infty) \\ &= (2m)(11) + + + [16m + 20n - 24] \\ &= 22m + 12m(n-2) + 24(n-1)(m-1) + 16m + 20n - 24 \\ &= 22m + 12mn - 24m + 24mn - 24m - 24n + 24 + 16m + 20n - 24 \\ &= 36mn - 10m - 4n. \end{aligned}$$

Now, for the special case when $m = 1$ (i.e., only one square per row), the structure consists of: - Internal faces: $|\varphi_{11}| = 2$, $|\varphi_{12}| = n - 2$ - External face: $\deg(\varphi_\infty) = 14n - 2$

Thus:

$$\begin{aligned} \mathbb{FI}(\mathcal{G}) &= 2(11) + (n-2)(12) + (14n - 2) \\ &= 22 + 12n - 24 + 14n - 2 \\ &= 26n - 4. \end{aligned}$$

Similarly, for $n = 1$, each row contains only one square. The structure has: - Only one type of internal face φ_{10}, with $|\varphi_{10}| = m$ - External face: $\deg(\varphi_\infty) = 10m + 2$

Hence:

$$\begin{aligned}\mathbb{FI}(\mathcal{G}) &= |\varphi_{10}|(10) + \deg(\varphi_\infty)\\ &= 10m + 10m + 2 = 20m + 2.\end{aligned}$$

This completes the proof.

Theorem 2.9 *Let $\mathcal{G}$ be the 2-dimensional lattice nanotorus $\mathcal{T}[m,n]$ with m squares in each row and n rows. Then the face index of $\mathcal{G}$ is given by:*

$$\mathbb{FI}(\mathcal{G}) = \begin{cases} 36mn - 4m - 4n, & \text{if } m,n > 1,\\ 26n + 2, & \text{if } m = 1,\\ 26m + 2, & \text{if } n = 1.\end{cases}$$

Proof: We analyze the face index of the 2D-lattice nanotorus structure $\mathcal{T}[m,n]$ by comparing it incrementally with the simpler nanotube and flat-lattice versions. According to previous theorem, the face index of the flat 2D-lattice structure $\mathcal{T}[m,n]$ (with open boundaries) is:

$$\mathbb{FI}_{\text{flat}} = 36mn - 10m - 10n.$$

Now, the nanotube structure $\mathcal{T}_{\text{tube}}[m,n]$ is constructed by connecting the left and right sides of the flat lattice, effectively forming a cylindrical topology. This wrapping adds $6n$ to the face index due to the insertion of extra edges along the column boundaries, as stated in Theorem 2.8. Thus, the face index for the nanotube is:

$$\mathbb{FI}_{\text{tube}} = \mathbb{FI}_{\text{flat}} + 6n = 36mn - 10m - 10n + 6n = 36mn - 10m - 4n.$$

Next, the nanotorus structure $\mathcal{T}[m,n]$ is formed by further connecting the top and bottom boundaries of the nanotube (completing the toroidal wrapping). This additional operation increases the face index by $6m$, resulting from the creation of m additional connections between rows. Therefore, the final face index becomes:

$$\mathbb{FI}_{\text{torus}} = \mathbb{FI}_{\text{tube}} + 6m = 36mn - 10m - 4n + 6m = 36mn - 4m - 4n.$$

Now, for the special case when $m = 1$, we use the same approach: - From Theorem 2.8, the face index for the nanotube when $m = 1$ is:

$$\mathbb{FI} = 26n - 4.$$

- Wrapping the top and bottom to form a nanotorus adds 6 units (since $6m = 6$ when $m = 1$), resulting in:

$$\mathbb{FI} = 26n - 4 + 6 = 26n + 2.$$

Similarly, for $n = 1$: - The face index of the nanotube with $n = 1$ is $20m+2$ - Adding $6n = 6$ increases the index to:

$$\mathbb{FI} = 20m + 2 + 6 = 26m + 2.$$

Hence, all three cases are verified, and this completes the proof.

3. Discussions and Graphical Analysis

This section discusses the computed results presented in Table 7 and interprets the trends exhibited by the graphical representations generated using the formulas derived in Theorems 1 to 9. The structures under investigation are based on the TUC_4C_8 lattice system, examined in three distinct forms: the original base structure $\mathcal{T}[3,n]$, its subdivision graph $\mathcal{S}(\mathcal{T}[3,n])$, and the line graph of the subdivision graph $\mathcal{L}_{\mathcal{S}}(\mathcal{T}[3,n])$. Each form is further extended into nanotube and nanotorus configurations. The analysis focuses on the face index as a structural invariant, computed for values of n ranging from 2 to 12 with a fixed number of square units in each row, $m = 3$. From the tabulated values, it is evident that

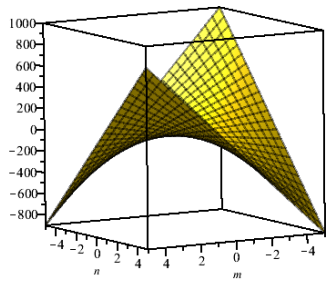
the face index grows steadily with increasing n across all graph types. For the base structure $\mathcal{T}[3,n]$, the face index starts at 164 for $n = 2$ and increases to 984 at $n = 12$, demonstrating a linear growth consistent with the analytical formula. When the structure is modified into a nanotube and nanotorus, the face index values also rise accordingly, but the nanotorus exhibits slightly higher values than the tube due to the additional edge connections introduced by its closed circular form. This effect highlights the influence of topological wrapping on face boundaries and vertex degrees.

The impact of subdivision is much more pronounced. The face index for the subdivision graph $\mathcal{S}(\mathcal{T}[3,n])$ is substantially higher compared to the base structure, with values ranging from 288 to 1728 as n varies from 2 to 12. This considerable increase is due to the new faces and vertices created during the subdivision process, which increase the total degree contributions across all faces. The tube and torus extensions of the subdivision graph also show similar increases, maintaining the order Base $<$ Tube $<$ Torus in terms of face index values at every level. The line graph of the subdivision graph, $\mathcal{L}_{\mathcal{S}}(\mathcal{T}[3,n])$, yields the highest face index values among all considered structures. Beginning from 584 at $n = 2$ and reaching 3504 at $n = 12$, these results confirm the compounding effects of subdivision followed by line graph transformation. The line graph operation transforms each edge into a vertex, thereby increasing the overall vertex-face adjacency and inflating the face index. The tube and torus versions of $\mathcal{L}_{\mathcal{S}}$ follow the same rising trend, with torus structures consistently yielding higher values due to increased connectivity at the boundaries.

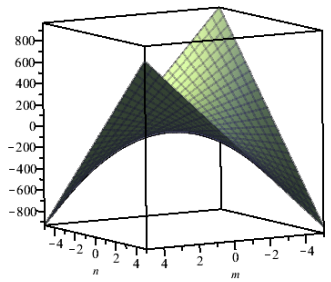
The graphical analysis, consisting of 3D surface plots generated from Theorems 1 to 9, visually confirms these trends. Each plot exhibits a smooth surface indicating linear or nearly linear relationships between the parameters m, n, and the resulting face index. In the figures corresponding to line graphs of subdivision graphs, the surface gradient is steeper, reflecting the rapid growth in face index. Moreover, the plots for nanotorus structures consistently lie above their tube and base counterparts, further reinforcing the observation that closed boundary conditions significantly affect face connectivity and complexity. In conclusion, both the tabulated results and the graphical trends clearly demonstrate that the face index is highly sensitive to structural modifications. Subdivision operations, followed by line graph transformations, substantially increase the structural complexity of the graph. The torus configuration amplifies this effect further due to its boundary-wrapping characteristics. These insights underscore the importance of the face index as a useful descriptor in the topological characterization of nanostructured graphs such as TUC_4C_8-based networks.

Structure ↓	2	3	4	5	6	7	8	9	10	11	12
$\mathcal{T}[3,n]$	164	246	328	410	492	574	656	738	820	902	984
Tube($\mathcal{T}$)	92	138	184	230	276	322	368	414	460	506	552
Torus($\mathcal{T}$)	104	168	232	296	360	424	488	552	616	680	744
$\mathcal{S}(\mathcal{T})$	288	432	576	720	864	1008	1152	1296	1440	1584	1728
Tube($\mathcal{S}$)	214	318	422	526	630	734	838	942	1046	1150	1254
Torus($\mathcal{S}$)	236	360	484	608	732	856	980	1104	1228	1352	1476
$\mathcal{L}_{\mathcal{S}}$	584	876	1168	1460	1752	2044	2336	2628	2920	3212	3504
Tube($\mathcal{L}_{\mathcal{S}}$)	428	642	856	1070	1284	1498	1712	1926	2140	2354	2568
Torus($\mathcal{L}_{\mathcal{S}}$)	500	732	964	1196	1428	1660	1892	2124	2356	2588	2820

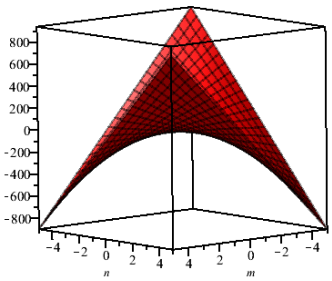
Table 7: Face index values for different structures derived from $\mathcal{T}[3,n]$ for $n = 2$ to 12.



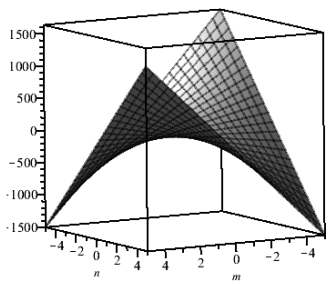
(a) Face Index of $\mathcal{T}[m,n]$ (Theorem 1)



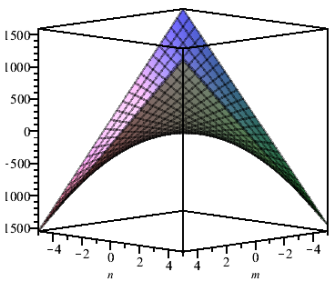
(b) Face Index of nanotube $\mathcal{T}[m,n]$ (Theorem 2)



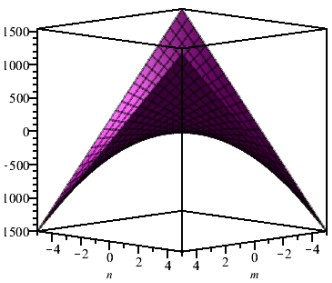
(c) Face Index of nanotorus $\mathcal{T}[m,n]$ (Theorem 3)



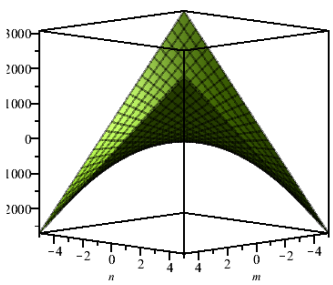
(d) Face Index of $\mathcal{S}(\mathcal{T}[m,n])$ (Theorem 4)



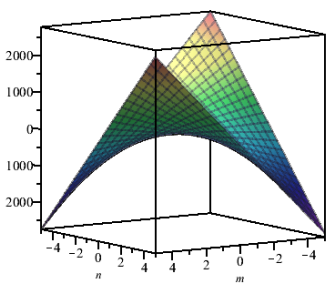
(e) Face Index of nanotube $\mathcal{S}(\mathcal{T}[m,n])$ (Theorem 5)



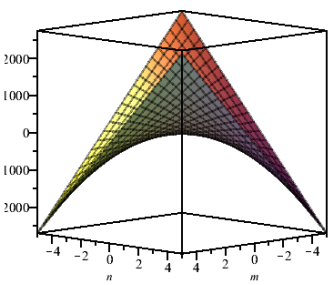
(f) Face Index of nanotorus $\mathcal{S}(\mathcal{T}[m,n])$ (Theorem 6)



(g) Face Index of $\mathcal{L}_{\mathcal{S}}(\mathcal{T}[m,n])$ (Theorem 7)



(h) Face Index of nanotube $\mathcal{L}_{\mathcal{S}}(\mathcal{T}[m,n])$ (Theorem 8)



(i) Face Index of nanotorus $\mathcal{L}_{\mathcal{S}}(\mathcal{T}[m,n])$ (Theorem 9)

Figure 5: 3D plots showing variation in face index $\mathbb{FI}(\mathcal{G})$ for different structural transformations of $\mathcal{T}[m,n]$ under Theorems 1 to 9.

4. Conclusion

In this study, we derived and analyzed explicit formulas for the face index of TUC_4C_8-based molecular graphs under various transformations, including subdivision and line graph operations. The computations were extended to their tube and torus configurations, and the resulting expressions provided insight into

how structural modifications impact the overall topological complexity of the graphs. By fixing the parameter $m = 3$ and varying n from 2 to 12, we compiled detailed face index values and compared them graphically. The results show a consistent and significant increase in the face index when moving from base to subdivision and from subdivision to line graph structures. Furthermore, nanotorus forms exhibit larger face indices than nanotube configurations due to the added vertex-face adjacencies introduced by the cyclic boundary conditions. The trends visualized in the 3D plots support the analytical findings and affirm the effectiveness of the face index as a structural descriptor. These observations not only contribute to the mathematical modeling of molecular lattices but also aid in understanding the geometric intricacies of complex nanostructures.

Declaration

- **Availabilty of data and materials:** The data is provided on request to the authors.
- **Authors Contribution:** All authors contributed equally in writing of this article.
- **Conflicts of interest:** The authors declare that they have no conflicts of interest and all agree to publish this paper under academic ethics.
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