

Neighborhood M-Polynomial of Crystallographic Structures

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Abstract: The mathematical chemistry is wealthy, having tools such as polynomials and functions that can predict the properties of compounds. The M-polynomial is one of them which yields degree-based topological indices. In this work, we define the neighborhood M-polynomial to obtain neighborhood degree-based topological indices. Further, we compute some neighborhood degree-based topological indices of the face-centered cubic (fcc) lattice and the crystallographic structure of cuprous oxide (Cu_2O) using the neighborhood M-polynomial approach. Also, the results are shown graphically.

Keywords: M-polynomial; Topological index; Face centered cubic (fcc) lattice; Crystallographic structure of cuprous oxide (Cu_2O).

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1. Introduction

We consider a connected graph having no loops and no parallel edges throughout this article. Let $V(G)$ and $E(G)$ be vertex set and edge set of a graph G , respectively. The total number of edges incident to $v \in V(G)$ is known as the degree of v and is denoted by d_v . Here δ_u denotes the degree sum of neighbors of u in G . By neighbors of a vertex, we mean the vertices adjacent to that vertex. Various physical properties, chemical reactivity, and biological activities of a molecule are strongly connected to its graphical structure, and this fact is the main topic of interest in chemical graph theory. The topological index plays a key role in predicting such a connection without involving a wet lab. A topological index is a function from the collection of graphs to the set of real numbers that describe the topology of the graph and are used in QSPR/QSAR analysis. It remains unchanged for isomorphic graphs. The idea of topological indices was initiated when the eminent chemist Harold Wiener found the first topological index, known as Wiener index [1] in 1947, for searching boiling points of alkanes. Then thousands of indices are developed in the literature of chemical graph theory. For some current works, readers are referred to [2-7].

Topological indices can be computed by their usual definitions, which is laborious, while one intends to derive many indices of a certain category. To overcome this approach, many algebraic polynomials [8-10] have been introduced whose differentiation or integration or blend of both, obtained at some particular point, give topological indices. The M-polynomial [11-16] is the most general polynomial to produce a large number of degree-based topological indices. Rapid advances are created on a day-to-day basis to design fresh indices. Recently, <https://biointerfaceresearch.com/>

some researchers put their attention on the neighborhood degree-based indices [17-24]. To make the computation of these types of indices easier, we introduce a polynomial named as neighborhood M-polynomial whose role for neighborhood degree-based indices is parallel to the role of the M-polynomial for degree-based indices. Thus from the neighborhood M-polynomial of a given family of graphs, its neighborhood degree-based indices can be recovered. Sometimes the function defining a topological index does not allow the neighborhood M-polynomial to obtain topological indices. In that case, equation (2) can be used to get the closed form of the neighborhood degree-based topological indices. The neighborhood M-polynomial of a graph G is defined as,

$$NM(G; x, y) = \sum_{i \leq j} m_{(i,j)} x^i y^j. \tag{1}$$

Where $m_{(i,j)}$ is the total number of edges $uv \in E(G)$ such that $\{\delta_u, \delta_v\} = \{i, j\}$. We use $NM(G)$ for $NM(G; x, y)$ for the rest of the article. The Neighborhood degree-based topological indices defined on the edge set of a graph G can be expressed as

$$I(G) = \sum_{uv \in E(G)} f(\delta_u, \delta_v),$$

where $f(\delta_u, \delta_v)$ is the function of δ_u, δ_v used in the definition of neighborhood degree-based indices. The above result can also be written as,

$$I(G) = \sum_{i \leq j} m_{(i,j)} f(i, j). \tag{2}$$

Now we describe some neighborhood degree-based topological indices.

The third version of the Zagreb index [21] is defined as,

$$M'_1(G) = \sum_{uv \in E(G)} (\delta_u + \delta_v).$$

The neighborhood second Zagreb index [19] is defined as,

$$M_2^*(G) = \sum_{uv \in E(G)} \delta_u \delta_v.$$

The neighborhood forgotten topological index [19] is defined as,

$$F_N^*(G) = \sum_{uv \in E(G)} (\delta_u^2 + \delta_v^2).$$

The neighborhood second modified Zagreb index is defined as,

$$M_2^{nm}(G) = \sum_{uv \in E(G)} \frac{1}{\delta_u \delta_v}.$$

The neighborhood general Randić index is defined as,

$$NR_\alpha(G) = \sum_{uv \in E(G)} (\delta_u \delta_v)^\alpha.$$

The third NDe index [20] is defined as,

$$ND_3(G) = \sum_{uv \in E(G)} \delta_u \delta_v (\delta_u + \delta_v).$$

The fifth NDe index [20] is defined as,

$$ND_5(G) = \sum_{uv \in E(G)} \left[\frac{\delta_u}{\delta_v} + \frac{\delta_v}{\delta_u} \right].$$

The neighborhood Harmonic index is defined as,

$$NH(G) = \sum_{uv \in E(G)} \frac{2}{\delta_u + \delta_v}.$$

The neighborhood inverse sum index is given by

$$NI(G) = \sum_{uv \in E(G)} \frac{\delta_u \delta_v}{\delta_u + \delta_v}.$$

The Sanskruti index [17] is defined as,

$$S(G) = \sum_{uv \in E(G)} \left(\frac{\delta_u \delta_v}{\delta_u + \delta_v - 2} \right)^3.$$

The relations of some neighborhood degree-based topological indices with the NM-polynomial are shown in Table 1.

Table 1. Derivation of some neighborhood degree-based topological indices.

Topological index	$f(x, y)$	Derivation from $NM(G)$
M_1'	$x + y$	$(D_x + D_y)(NM(G)) _{x=y=1}$
M_2^*	xy	$(D_x D_y)(NM(G)) _{x=y=1}$
F_N^*	$x^2 + y^2$	$(D_x^2 + D_y^2)(NM(G)) _{x=y=1}$
M_2^{nm}	$\frac{1}{xy}$	$(S_x S_y)(NM(G)) _{x=y=1}$
NR_α	$(xy)^\alpha$	$(D_x^\alpha D_y^\alpha)(NM(G)) _{x=y=1}$
ND_3	$xy(x+y)$	$D_x D_y (D_x + D_y)(NM(G)) _{x=y=1}$
ND_5	$\frac{x^2 + y^2}{xy}$	$(D_x S_y + S_x D_y)(NM(G)) _{x=y=1}$
NH	$\frac{2}{x+y}$	$2S_x J(NM(G)) _{x=y=1}$
NI	$\frac{xy}{x+y}$	$S_x J D_x D_y (NM(G)) _{x=y=1}$
S	$\frac{xy}{(x+y-2)^3}$	$S_x^3 Q_{-2} J D_x^3 D_y^3 (NM(G)) _{x=y=1}$

Where,

$$D_x(f(x, y)) = x \frac{\partial(f(x,y))}{\partial x}, \quad D_y(f(x, y)) = y \frac{\partial(f(x,y))}{\partial y}, \quad S_x(f(x, y)) = \int_0^x \frac{f(t,y)}{t} dt,$$

$$S_y(f(x, y)) = \int_0^y \frac{f(x,t)}{t} dt, \quad J(f(x, y)) = f(x, x), \quad Q_\alpha(f(x, y)) = x^\alpha f(x, y).$$

Digital geometry deals with graphs with regular, periodic constructions and is strongly associated with crystallography in this manner. It is also applicable in image processing and computer graphics. One of the main directions of research of digital geometry deals with 3D grids and crystallographic structures. In this article, we intend to derive some neighborhood degree-based indices of face-centered cubic lattice and the crystallographic structure of cuprous oxide (Cu_2O).

Face centered cubic lattice [25, 26] is constructed by cubic unit cells having an atom at each corner of the cube and an atom at the center of each face of the cube (Figure 1). Edges connect the closest atoms. This structure has the largest packing density in three-dimensional space. Copper, aluminum, nickel, silver, and gold are some of the materials with a fcc framework. Here we consider the lines of unit cells of the cross-section of fcc lattice (i.e., the dimension of our space is $n \times 1 \times 1$ unit cells). Cuprous oxide [27, 28, 29], a p-type semiconductor with distinctive optical and magnetic characteristics, can be used in the transformation for solar energy, electronics, magnetic storage, catalysis, and gas sensors. The crystallographic structure of Cu_2O , depicted in Figure 3, consists of $m \times n$ units in the mn-plane and then storing it up in t layers.

2. Materials and Methods

Our main computational results include some neighborhood degree sum based indices of centered cubic lattice and crystallographic structure of cuprous oxide via the NM-polynomial approach. To compute our results, we used the method of combinatorial computing, edge partition method, and graph-theoretical tools. First of all, we compute NM-polynomial. Then using some calculus operators, we recover the topological indices from those NM-polynomials. The graphical representations of the outcomes are shown using Maple 2015.

3. Results and Discussion

In this part, we give our main computational results and divide the section into two subsections.

3.1. Computational aspects of the face-centered cubic lattice.

We compute the NM-polynomial of face-centered cubic lattice in the following theorem.

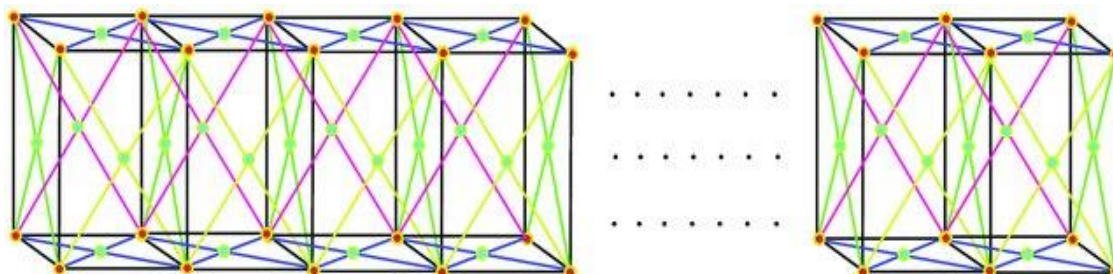


Figure 1. Face centered cubic lattice (fcc(n)).

Theorem 1. Let G be the face-centered cubic lattice (fcc(n)). Then we have,

$$NM(G) = 8x^{24}y^{33} + 16x^{30}y^{33} + 16x^{30}y^{53} + 8x^{33}y^{33} + 8x^{33}y^{53} + 24x^{36}y^{53} + 20(n-3)x^{36}y^{56} + 8x^{53}y^{53} + 8x^{53}y^{56} + 4(2n-7)x^{56}y^{56}.$$

Proof. The fcc lattice has $28n + 8$ number of edges. Its edge set can be partitioned as follows:

$$\begin{aligned} |E_{\{24,33\}}| &= |\{uv \in E(G) : \delta_u = 24, \delta_v = 33\}| = 8 = m_{(24,33)}, \\ |E_{\{30,33\}}| &= |\{uv \in E(G) : \delta_u = 30, \delta_v = 33\}| = 16 = m_{(30,33)}, \\ |E_{\{30,53\}}| &= |\{uv \in E(G) : \delta_u = 30, \delta_v = 53\}| = 16 = m_{(30,53)}, \\ |E_{\{33,33\}}| &= |\{uv \in E(G) : \delta_u = 33, \delta_v = 33\}| = 8 = m_{(33,33)}, \\ |E_{\{33,53\}}| &= |\{uv \in E(G) : \delta_u = 33, \delta_v = 53\}| = 8 = m_{(33,53)}, \\ |E_{\{36,53\}}| &= |\{uv \in E(G) : \delta_u = 36, \delta_v = 33\}| = 24 = m_{(36,53)}, \\ |E_{\{36,56\}}| &= |\{uv \in E(G) : \delta_u = 36, \delta_v = 56\}| = 20(n-3) = m_{(36,56)}, \\ |E_{\{53,53\}}| &= |\{uv \in E(G) : \delta_u = 53, \delta_v = 53\}| = 8 = m_{(53,53)}, \\ |E_{\{53,56\}}| &= |\{uv \in E(G) : \delta_u = 53, \delta_v = 56\}| = 8 = m_{(53,56)}, \\ |E_{\{56,56\}}| &= |\{uv \in E(G) : \delta_u = 56, \delta_v = 56\}| = 4(2n-7) = m_{(56,56)}. \end{aligned}$$

From the definition, the NM-polynomial of G is obtained bellow.

$$\begin{aligned} NM(G) &= \sum_{i \leq j} m_{(i,j)} x^i y^j \\ &= m_{(24,33)} x^{24} y^{33} + m_{(30,33)} x^{30} y^{33} + m_{(30,53)} x^{30} y^{53} + m_{(33,33)} x^{33} y^{33} \\ &\quad + m_{(33,53)} x^{33} y^{53} + m_{(36,53)} x^{36} y^{53} + m_{(36,56)} x^{36} y^{56} \\ &\quad + m_{(53,53)} x^{53} y^{53} + m_{(53,56)} x^{53} y^{56} + m_{(56,56)} x^{56} y^{56} \\ &= 8x^{24}y^{33} + 16x^{30}y^{33} + 16x^{30}y^{53} + 8x^{33}y^{33} + 8x^{33}y^{53} + 24x^{36}y^{53} + \\ &\quad 20(n-3)x^{36}y^{56} + 8x^{53}y^{53} + 8x^{53}y^{56} + 4(2n-7)x^{56}y^{56} \end{aligned}$$

This completes the proof.

Now using this NM-polynomial, we calculate some neighborhood degree-based topological indices of the face-centered cubic lattice in the following theorem.

Theorem 2. Let G be the face-centered cubic lattice (fcc(n)). Then we have,

1. $M'_1(G) = 2736n - 792,$

2. $M_2^*(G) = 65408n - 46440,$
3. $F_N^*(G) = 138816n - 97416,$
4. $M_2^{nm}(G) = 0.012n + 0.028,$
5. $NR_\alpha(G) = 8(792)^\alpha + 16(990)^\alpha + 16(1590)^\alpha + 8(33)^{2\alpha} + 8(1749)^\alpha + 24(1908)^\alpha + 20(n - 3)(2016)^\alpha + 8(53)^{2\alpha} + 8(2968)^\alpha + 4(2n - 7)(56)^{2\alpha},$
6. $ND_3(G) = 6519296n - 6668304,$
7. $ND_5(G) = 59.968n + 15.871,$
8. $NH(G) = 0.578n + 0.636,$
9. $NI(G) = 662.261n - 190.641,$
10. $S(G) = 410158.754n - 416703.851.$

Proof. Let $NM(G) = f(x, y) = 8x^{24}y^{33} + 16x^{30}y^{33} + 16x^{30}y^{53} + 8x^{33}y^{33} + 8x^{33}y^{53} + 24x^{36}y^{53} + 20(n - 3)x^{36}y^{56} + 8x^{53}y^{53} + 8x^{53}y^{56} + 4(2n - 7)x^{56}y^{56}.$

Then we have,

$$(D_x + D_y)(f(x, y)) = 456x^{24}y^{33} + 1008x^{30}y^{33} + 1328x^{30}y^{53} + 528x^{33}y^{33} + 688x^{33}y^{53} + 2136x^{36}y^{53} + 1840(n - 3)x^{36}y^{56} + 848x^{53}y^{53} + 872x^{53}y^{56} + 448(2n - 7)x^{56}y^{56},$$

$$(D_x D_y)(f(x, y)) = 6336x^{24}y^{33} + 15840x^{30}y^{33} + 25440x^{30}y^{53} + 8712x^{33}y^{33} + 13992x^{33}y^{53} + 45792x^{36}y^{53} + 40320(n - 3)x^{36}y^{56} + 22472x^{53}y^{53} + 23744x^{53}y^{56} + 12544(2n - 7)x^{56}y^{56},$$

$$(D_x^2 + D_y^2)(f(x, y)) = 13320x^{24}y^{33} + 31824x^{30}y^{33} + 59344x^{30}y^{53} + 17424x^{33}y^{33} + 31184x^{33}y^{53} + 98520x^{36}y^{53} + 88640(n - 3)x^{36}y^{56} + 44944x^{53}y^{53} + 47560x^{53}y^{56} + 25088(2n - 7)x^{56}y^{56},$$

$$S_x S_y(f(x, y)) = \frac{1}{99}x^{24}y^{33} + \frac{8}{495}x^{30}y^{33} + \frac{8}{795}x^{30}y^{53} + \frac{8}{1089}x^{33}y^{33} + \frac{8}{1749}x^{33}y^{53} + \frac{2}{159}x^{36}y^{53} + \frac{5(n-3)}{504}x^{36}y^{56} + \frac{8}{2809}x^{53}y^{53} + \frac{8}{2968}x^{53}y^{56} + \frac{2n-7}{784}x^{56}y^{56},$$

$$D_x^\alpha D_y^\alpha(f(x, y)) = 8(792)^\alpha x^{24}y^{33} + 16(990)^\alpha x^{30}y^{33} + 16(1590)^\alpha x^{30}y^{53} + 8(33)^{2\alpha} x^{33}y^{33} + 8(1749)^\alpha x^{33}y^{53} + 24(1908)^\alpha x^{36}y^{53} + 20(n - 3)(2016)^\alpha x^{36}y^{56} + 8(53)^{2\alpha} x^{53}y^{53} + 8(2968)^\alpha x^{53}y^{56} + 4(2n - 7)(56)^{2\alpha} x^{56}y^{56},$$

$$D_x D_y(D_x + D_y)(f(x, y)) = 361152x^{24}y^{33} + 997920x^{30}y^{33} + 2111520x^{30}y^{53} + 574992x^{33}y^{33} + 1203312x^{33}y^{53} + 4075488x^{36}y^{53} + 3709440(n - 3)x^{36}y^{56} + 2382032x^{53}y^{53} + 2588096x^{53}y^{56} + 1404928(2n - 7)x^{56}y^{56},$$

$$(D_x S_y + S_x D_y)(f(x, y)) = \frac{1665}{99}x^{24}y^{33} + \frac{15912}{495}x^{30}y^{33} + \frac{29672}{795}x^{30}y^{53} + 16x^{33}y^{33} + \frac{31184}{1749}x^{33}y^{53} + \frac{8210}{159}x^{36}y^{53} + \frac{22160(n-3)}{504}x^{36}y^{56} + 16x^{53}y^{53} + \frac{5945}{371}x^{53}y^{56} + 8(2n - 7)x^{56}y^{56},$$

$$S_x J(f(x, y)) = \frac{8}{57}x^{57} + \frac{16}{63}x^{63} + \frac{16}{83}x^{83} + \frac{4}{33}x^{66} + \frac{4}{43}x^{86} + \frac{24}{89}x^{89} + \frac{5(n-3)}{23}x^{92} + \frac{4}{53}x^{106} + \frac{8}{109}x^{109} + \frac{2n-7}{28}x^{112},$$

$$S_x J D_x D_y(f(x, y)) = \frac{6336}{57}x^{57} + \frac{15840}{63}x^{63} + \frac{25440}{83}x^{83} + \frac{4356}{33}x^{66} + \frac{6996}{43}x^{86} + \frac{45792}{89}x^{89} + \frac{10080(n-3)}{23}x^{92} + \frac{11236}{53}x^{106} + \frac{23744}{109}x^{109} + \frac{3136(2n-7)}{28}x^{112},$$

$$S_x^3 Q_{-2} J D_x^3 D_y^3(f(x, y)) = 23887.872x^{55} + 68396.844x^{61} + 121019.763x^{81} + 39412.475x^{64} + 72214.026x^{84} + 253156.216x^{87} + 224788.48(n - 3)x^{90} + 157632.291x^{104} + 170738.061x^{107} + 92685.137(2n - 7)x^{110}.$$

Using Table 1, we can easily obtain the required result.

The topological indices of the face-centered cubic lattice are depicted in Figure 2.

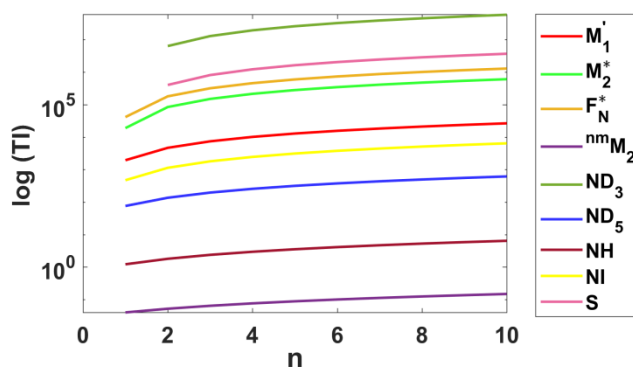


Figure 2. Topological indices of a face-centered cubic lattice (fcc(n)). By log(TI), we mean logarithm of topological indices.

3.2. Computational aspects of the crystallographic structure of $Cu_2O[m, n, t]$.

We compute the NM-polynomial of the crystallographic structure of $Cu_2O[m, n, t]$ in the following theorem.

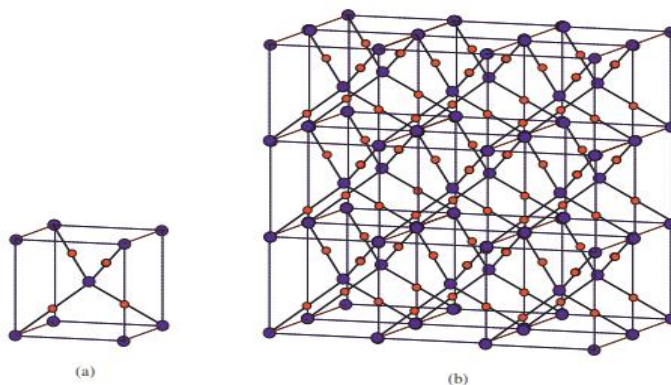


Figure 3. (a) Unit cell of Cu_2O [1,1,1] (b) Crystallographic structure of Cu_2O [3,2,3].

Theorem 3. Let G be the crystallographic structure of $Cu_2O[m, n, t]$. Then we have

$$NM(G) = 4(m + n + t - 2)x^2y^4 + 4(mn + mt + nt - 2m - 2n - 2t + 3)x^4y^6 + 4(m + n + t - 2)x^5y^8 + 4(mn + mt + nt - 2m - 2n - 2t + 3)x^6y^8 + 8(mnt - mn - mt - nt + m + n + t - 1)x^8y^8.$$

Proof. The crystallographic structure of $Cu_2O[m, n, t]$ has $8mnt$ number of edges. Its edge set has partitions as follows:

$$|E_{\{2,4\}}| = |\{uv \in E(G) : \delta_u = 2, \delta_v = 4\}| = 4(m + n + t - 2) = m_{(2,4)},$$

$$|E_{\{4,6\}}| = |\{uv \in E(G) : \delta_u = 4, \delta_v = 6\}| = 4(mn + mt + nt - 2m - 2n - 2t + 3) = m_{(4,6)},$$

$$|E_{\{5,8\}}| = |\{uv \in E(G) : \delta_u = 5, \delta_v = 8\}| = 4(m + n + t - 2) = m_{(5,8)},$$

$$|E_{\{6,8\}}| = |\{uv \in E(G) : \delta_u = 6, \delta_v = 8\}| = 4(mn + mt + nt - 2m - 2n - 2t + 3) = m_{(6,8)},$$

$$|E_{\{8,8\}}| = |\{uv \in E(G) : \delta_u = 8, \delta_v = 8\}| = 8(mnt - mn - mt - nt + m + n + t - 1) = m_{(8,8)}.$$

From the definition, the NM-polynomial of G is obtained bellow,

$$NM(G) = \sum_{i \leq j} m_{(i,j)} x^i y^j$$

$$\begin{aligned}
 &= m_{(2,4)}x^2y^4 + m_{(4,6)}x^4y^6 + m_{(5,8)}x^5y^8 + m_{(6,8)}x^6y^8 + m_{(8,8)}x^8y^8 \\
 &= 4(m+n+t-2)x^2y^4 + 4(mn+mt+nt-2m-2n-2t+3)x^4y^6 \\
 &\quad + 4(m+n+t-2)x^5y^8 + 4(mn+mt+nt-2m-2n-2t+3)x^6y^8 \\
 &\quad + 8(mnt-mn-mt-nt+m+n+t-1)x^8y^8.
 \end{aligned}$$

This completes the proof.

The surface representations of NM-polynomials of both the structures are shown in Figure 4.

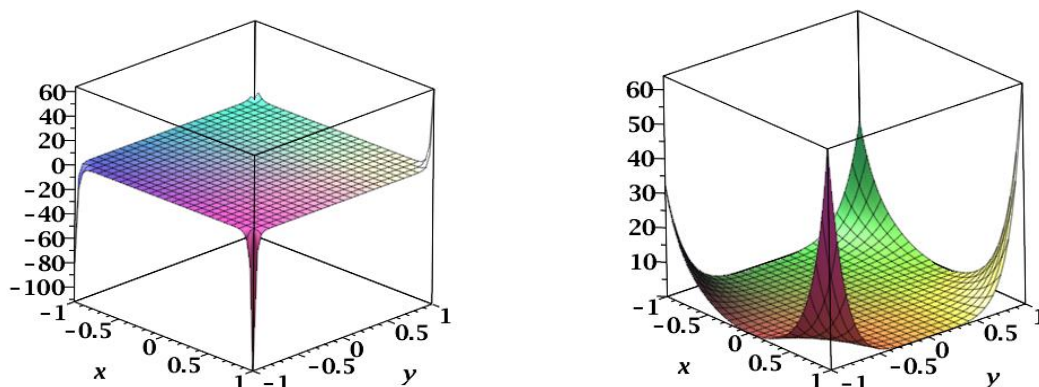


Figure 4. The NM-polynomial of (a) the face-centered cubic lattice for $n=2$ and (b) the $Cu_2O[2,2,2]$.

Now using this *NM*-polynomial, we calculate some degree-based topological indices of the crystallographic structure of $Cu_2O[m, n, t]$ in the following theorem.

Theorem 4. Let G be the crystallographic structure of $Cu_2O[m, n, t]$. Then we have,

1. $M'_1(G) = 128mnt - 32mn - 32mt - 32nt + 68m + 68n + 68t + 8,$
2. $M_2^*(G) = 512mnt - 224mn - 224mt - 224nt + 128m + 128n + 128t - 32,$
3. $F_N^*(G) = 1024mnt - 416mn - 416mt - 416nt + 244m + 244n + 244t - 72,$
4. $M_2^{nm}(G) = \frac{1}{8}mnt - \frac{1}{8}mn - \frac{1}{8}mt - \frac{1}{8}nt + \frac{47}{120}m + \frac{47}{120}n + \frac{47}{120}t - \frac{23}{40},$
5. $NR_\alpha(G) = 2^{3\alpha+2}(m+n+t-2) + 2^{3\alpha+2}3^\alpha(mn+mt+nt-2m-2n-2t+3) + 2^{3\alpha+2}5^\alpha(m+n+t-2) + 2^{4\alpha+2}3^\alpha(mn+mt+nt-2m-2n-2t+3) + 2^{6\alpha+3}(mnt-mn-mt-nt+m+n+t-1),$
6. $ND_3(G) = 8192mnt - 4544mn - 4544mt - 4544nt + 2976m + 2976n + 2976t - 9600,$
7. $ND_5(G) = 16mnt + mn + mt + nt + \frac{9}{10}m + \frac{9}{10}n + \frac{9}{10}t - \frac{14}{5},$
8. $NH(G) = mnt + \frac{13}{35}mn + \frac{13}{35}mt + \frac{13}{35}nt + \frac{221}{1365}m + \frac{221}{1365}n + \frac{221}{1365}t - \frac{1069}{1365},$
9. $NI(G) = 32mnt - \frac{304}{35}mn - \frac{304}{35}mt - \frac{304}{35}nt + \frac{4112}{1365}m + \frac{4112}{1365}n + \frac{4112}{1365}t - \frac{3632}{1365},$
10. $S(G) = 764.268mnt - 400.268mn - 400.268mt - 400.268nt + 260.604m + 260.604n + 260.604t - 120.94.$

Proof. Let $NM(G) = f(x, y) = 4(m+n+t-2)x^2y^4 + 4(mn+mt+nt-2m-2n-2t+3)x^4y^6 + 4(m+n+t-2)x^5y^8 + 4(mn+mt+nt-2m-2n-2t+3)x^6y^8 + 8(mnt-mn-mt-nt+m+n+t-1)x^8y^8.$

Then we have,

$$\begin{aligned}
 (D_x + D_y)(f(x, y)) &= 24(m+n+t-2)x^2y^4 + 40(mn+mt+nt-2m-2n-2t+3)x^4y^6 \\
 &+ 52(m+n+t-2)x^5y^8 + 56(mn+mt+nt-2m-2n-2t+3)x^6y^8 + \\
 &128(mnt-mn-mt-nt+m+n+t-1)x^8y^8,
 \end{aligned}$$

$$\begin{aligned}
 (D_x D_y)(f(x, y)) &= 32(m + n + t - 2)x^2 y^4 + 96(mn + mt + nt - 2m - 2n - 2t + 3)x^4 y^6 + 160(m + n + t - 2)x^5 y^8 + 192(mn + mt + nt - 2m - 2n - 2t + 3)x^6 y^8 + 512(mnt - mn - mt - nt + m + n + t - 1)x^8 y^8, \\
 (D_x^2 + D_y^2)(f(x, y)) &= 80(m + n + t - 2)x^2 y^4 + 208(mn + mt + nt - 2m - 2n - 2t + 3)x^4 y^6 + 356(m + n + t - 2)x^5 y^8 + 400(mn + mt + nt - 2m - 2n - 2t + 3)x^6 y^8 + 1024(mnt - mn - mt - nt + m + n + t - 1)x^8 y^8, \\
 S_x S_y(f(x, y)) &= \frac{1}{2}(m + n + t - 2)x^2 y^4 + \frac{1}{6}(mn + mt + nt - 2m - 2n - 2t + 3)x^4 y^6 + \frac{1}{10}(m + n + t - 2)x^5 y^8 + \frac{1}{12}(mn + mt + nt - 2m - 2n - 2t + 3)x^6 y^8 + \frac{1}{8}(mnt - mn - mt - nt + m + n + t - 1)x^8 y^8, \\
 D_x^\alpha D_y^\alpha(f(x, y)) &= 2^{3\alpha+2}(m + n + t - 2)x^2 y^4 + 2^{3\alpha+2}3^\alpha(mn + mt + nt - 2m - 2n - 2t + 3)x^4 y^6 + 2^{3\alpha+2}5^\alpha(m + n + t - 2)x^5 y^8 + 2^{4\alpha+2}3^\alpha(mn + mt + nt - 2m - 2n - 2t + 3)x^6 y^8 + 2^{6\alpha+3}(mnt - mn - mt - nt + m + n + t - 1)x^8 y^8, \\
 D_x D_y(D_x + D_y)(f(x, y)) &= 192(m + n + t - 2)x^2 y^4 + 960(mn + mt + nt - 2m - 2n - 2t + 3)x^4 y^6 + 2080(m + n + t - 2)x^5 y^8 + 2688(mn + mt + nt - 2m - 2n - 2t + 3)x^6 y^8 + 8192(mnt - mn - mt - nt + m + n + t - 1)x^8 y^8, \\
 (D_x S_y + S_x D_y)(f(x, y)) &= 10(m + n + t - 2)x^2 y^4 + \frac{26}{3}(mn + mt + nt - 2m - 2n - 2t + 3)x^4 y^6 + \frac{89}{10}(m + n + t - 2)x^5 y^8 + \frac{25}{3}(mn + mt + nt - 2m - 2n - 2t + 3)x^6 y^8 + 16(mnt - mn - mt - nt + m + n + t - 1)x^8 y^8, \\
 S_x J(f(x, y)) &= \frac{2}{3}(m + n + t - 2)x^6 + \frac{2}{5}(mn + mt + nt - 2m - 2n - 2t + 3)x^{10} + \frac{4}{13}(m + n + t - 2)x^{13} + \frac{2}{7}(mn + mt + nt - 2m - 2n - 2t + 3)x^{14} + \frac{1}{2}(mnt - mn - mt - nt + m + n + t - 1)x^{16}, \\
 S_x J D_x D_y(f(x, y)) &= \frac{16}{3}(m + n + t - 2)x^6 + \frac{48}{5}(mn + mt + nt - 2m - 2n - 2t + 3)x^{10} + \frac{160}{13}(m + n + t - 2)x^{13} + \frac{96}{7}(mn + mt + nt - 2m - 2n - 2t + 3)x^{14} + 32(mnt - mn - mt - nt + m + n + t - 1)x^{16}, \\
 S_x^3 Q_{-2} J D_x^3 D_y^3(f(x, y)) &= 32(m + n + t - 2)x^4 + 108(mn + mt + nt - 2m - 2n - 2t + 3)x^8 + 192.336(m + n + t - 2)x^{11} + 256(mn + mt + nt - 2m - 2n - 2t + 3)x^{12} + 764.268(mnt - mn - mt - nt + m + n + t - 1)x^{14}.
 \end{aligned}$$

Using Table 1, we can easily obtain the required result.

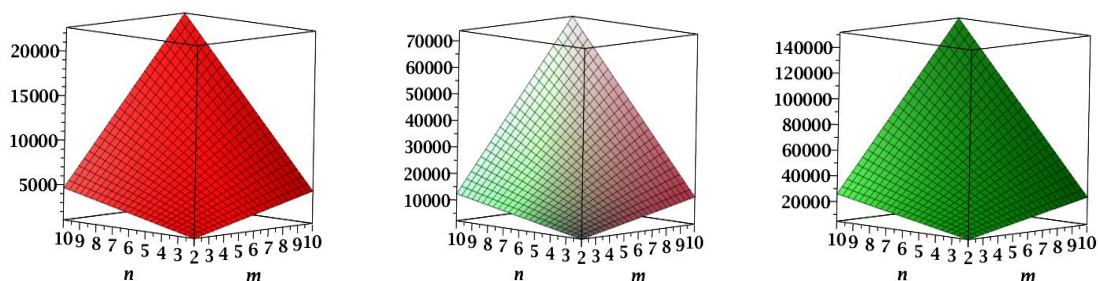


Figure 5. (a) M'_1 , (b) M_2^* , and (c) F_N^* index of $Cu_2O[m, n, 2]$.

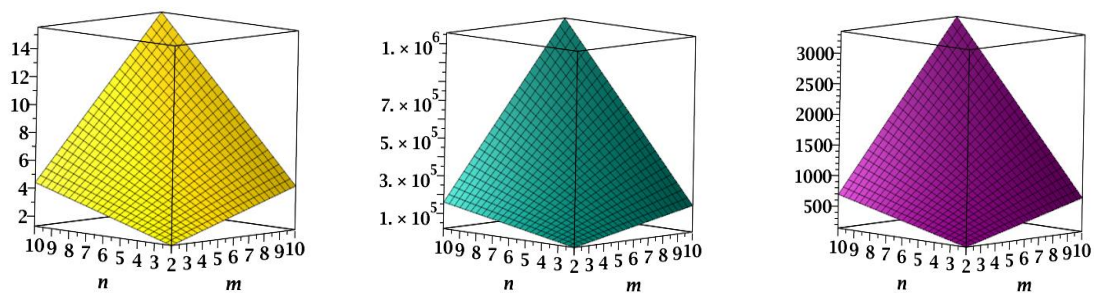


Figure 6. (a) M_2^{nm} , (b) ND_3 , and (c) ND_5 index of $Cu_2O[m, n, 2]$.

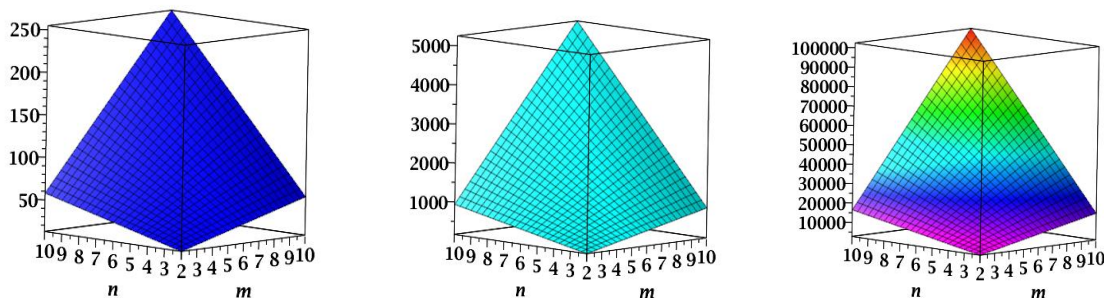


Figure 7. (a) NH , (b) NI , and (c) S index of $Cu_2O[m, n, 2]$.

The topological indices of the crystallographic structure of $Cu_2O[m, n, t]$ are depicted in Figure 4, Figure 5, and Figure 6.

4. Conclusions

In this article, we defined neighborhood M-polynomial to recover neighborhood degree-based topological indices. Here we considered the face-centered cubic lattice and the crystallographic structure of Cu_2O . Firstly, the general form of neighborhood M-polynomial for the structures is obtained and then using that polynomial, some neighborhood degree-based indices are recovered. To visualize the results, their graphical representation also has been made. These results can be helpful in understanding the typologies of the aforesaid structures.

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Conflicts of Interest

The authors declare no conflict of interest.

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