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On Degree Based Topological Indices of TiO_2 Crystal via M-Polynomial

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Abstract

Topological indices (TI) (descriptors) of a molecular graph are very much useful to study various physiochemical properties. It is also used to develop the quantitative structure-activity relationship (QSAR), quantitative structure-property relationship (QSPR) of the corresponding chemical compound. Various techniques have been developed to calculate the TI of a graph. Recently a technique of calculating degree-based TI from M-polynomial has been introduced. We have evaluated various topological descriptors for 3-dimensional TiO_2 crystals using M-polynomial. These descriptors are constructed such that it contains 3 variables (m, n and t) each corresponding to a particular direction. These 3 variables facilitate us to deeply understand the growth of TiO_2 in 1 dimension (1D), 2 dimensions (2D), and 3 dimensions (3D) respectively.

Keywords: Topological index, M-polynomial, TiO_2, Crystal, Chemical graph

Introduction

Mathematical chemistry is an inseparable part of material science. Here, we analyze some material structures using various mathematical techniques. This technique involves the well-established branch of mathematics known as graph theory. We apply the ideas of graph theory to conceptualize material science mathematically. These studies are also known as molecular graphs [1,2]. A molecular graph is a simple graph in which the edges denote the chemical bonding while vertices denote the atoms in a given material structure [3]. Gao *et al.* [4] discussed various TI w.r.t a family of anticancer drugs. These anticancer drugs are different kinds of polymers. Wu *et al.* [5] studied properties of nanostardendrimer and V-phenylenicnanotorous via TI. Shirakol *et al.* [6] calculated various TI of 68 types of Alkanes. They tried to establish a relation between different physical variables such as boiling point, melting point, heats of vaporization, etc. Kang *et al.* [7] computed TI of some organic compounds which can be further utilized to predict properties such as boiling point. Zhen-dong *et al.* [8] calculated 1 TI for the system such as saturated hydrocarbons, unsaturated hydrocarbons, oxygenic organic, methane halide and transition element compounds. Recently, Arockiaraj *et al.* [9] investigated distance based TI of nanosheets, nanotubes and nanotori of SiO_2. Also, Arockiaraj *et al.* [10] made a study on distance-based and degree-distance based TIs of pruned quartz and its related structures. All the structures discussed by them are of 2D, i.e., layer structure. Randic *et al.* [11] computed TI for several number of alkanes. Mujahed and Nagy [12] calculated the Wiener index (a type of TI) of the unit cell of body centered cubic (bcc) system. They studied the TI for the bcc system connected row wise. Kwun *et al.* [13] investigated TI of 2 Boron nanotube. This is also an example of 2D structure. Munir *et al.* [14] discussed M-polynomials of a single-walled TiO_2 nanotube. They computed some of the TI of a 2D, 6 layered single-walled TiO_2 nanotube.

Recently, Kaatz *et al.* [15] worked on various structures of clusters and calculated different TI for those. They worked on a total of 19 cluster types. There, the study was focused on clusters with a variety of layers in them. The study was on 1D structures.

From the literature survey, it is observed that the most of computation of indices is basically done for hydrocarbon and 2D systems. Baig *et al.* [16] and Yang *et al.* [17] investigated crystal cubic carbon and TiF_2, Copper (I) Oxide respectively. Both these works are done on 3D systems. Though, both the work did not construct 'M-polynomial'. In this system, a degree-based TI can be expressed as derivatives or integrals (sometimes both) of the corresponding M-polynomial [18]. This implies that any degree-based TI can be obtained from the constructed M-polynomial. The method of calculation of TI through M-polynomial consumes less computing time.

TiO_2 is a highly investigated wide band gap semiconductor owing to its excellent structural stability and enormous applications [19]. Two of the many applications of TiO_2 are photocatalytic activity and solar cell [20]. These 2 properties are highly dependent on the structural configuration of TiO_2. Other physical properties of TiO_2 such as optical activity [21,22], Electrical [23], magnetic [24], bioactivity [25,26] are also dependent on the size and structural configuration of TiO_2. The basic definition of crystal asks the system's smallest unit to be periodic, 3D, and infinite but nothing is infinite and hence diverges from the identical behavior of crystal. All the physical properties somehow become dependent on the number of repetitions; which can be in 1D, 2D, or 3D.

In this work, we have constructed M-polynomials and from it derived TI such as 1st Zagreb index, 2nd Zagreb index, 2nd Modified Zagreb index, General Randic index, General Inverse Randic index, Symmetric division index (SDD), harmonic index, inverse sum index and augmented Zagreb index for TiO_2 crystal in 3D. These indices will show different variations with the increment of TiO_2 unit cells in 3D. We are defining these mathematical indices for TiO_2 crystal and studied their variation with the increment of size along with 1D, 2D, or 3D. These variations of indices can be correlated with any size-dependent physical property.

Topological indices via M-polynomial

In Chemical graph theory, numerous graph polynomials have been introduced such as Hosoya polynomial [27], Zhang-Zhang or Clar covering polynomial [28], matching polynomial [29], Schultz polynomial [30], Tutte polynomial [31], Omega polynomial [32], etc. In 2015, Deutsch and Klavzar have introduced the M-polynomial [18]. Since then, it has been used by various researchers [14,33-35] to calculate TI of molecular graphs.

Let $G = (V, E)$ be a simple connected graph with vertex set $V(G)$ and edge set $E(G)$, d_u denotes the degree of the vertex $u \in V(G)$.Then, the M-polynomial of the graph G is defined as [18]:

$$M(G; x, y) = \sum_{\delta \le i \le j \le \Delta} m_{ij}(G) x^i y^j$$

Where $m_{ij}(G)$is the number of edges $uv \in E(G)$ such that $\{d_u, d_v\} = \{i, j\}$, $\delta = \min\{d_v | v \in V(G)\}$, and $\Delta = \max\{d_v | v \in V(G)\}$.

The 1st topological index was defined by Wiener [36] in 1947, which is known as the Wiener index. This distance-based topological index has many famous mathematical and chemical applications [36,37]. In 1975 Milan Randic proposed and formulated the Randic index of a graph G denoted by $R_{-(1/2)}(G)$.

$$R_{-(1/2)}(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_u d_v}}$$

In 1998 working independently by Bollobas and Erdos [37] and Amic *et al.* [38] generalized the concept of the Randic index and defined 'The General Randic index'. It is the most popular and most studied topological index. It has many useful applications in Chemistry, especially in drug design. For a graph G the General Randic index and General Inverse Randic index are formulated as:

$$R_\alpha(G) = \sum_{uv \in E(G)} (d_u d_v)^\alpha$$

$$RR_\alpha(G) = \sum_{uv \in E(G)} \frac{1}{(d_u d_v)^\alpha}$$

Gutman and Trinajstic introduced the 1st and 2nd Zagreb indices [39-41]. Both 1st and 2nd Zagreb indices along with the 2nd modified Zagreb index are defined as:

$$M_1(G) = \sum_{uv\in E(G)} (d_u + d_v)$$
$$M_2(G) = \sum_{uv\in E(G)} (d_u d_v)$$

$$m_{M_2}(G) = \sum_{uv\in E(G)} \frac{1}{d_u d_v}$$

Recently, the SDD of a connected graph G is introduced [42]. Which is a good predictor of the total surface area of polychlorobiphenyls [43] and is defined as:

$$SDD(G) = \sum_{uv\in E(G)} \left(\frac{\min(d_u, d_v)}{\max(d_u, d_v)} + \frac{\max(d_u, d_v)}{\min(d_u, d_v)}\right)$$

The Harmonic index [44] of a graph G which is another version of the Randic index is defined as:

$$H(G) = \sum_{uv\in E(G)} \frac{2}{d_u + d_v}$$

The Inverse sum index [45] of a graph G, which is a significant predictor of the total surface area of octane isomers [46], is defined as:

$$I(G) = \sum_{uv\in E(G)} \frac{d_u d_v}{d_u + d_v}$$

The augmented Zagreb index proposed by Furtula *et al*. [47] gives best approximation of the heat of formation of alkanes [47,48]. It is formulated as:

$$A(G) = \sum_{uv\in E(G)} \left(\frac{d_u d_v}{d_u + d_v - 2}\right)^3$$

Let $M(G; x, y) = f(x, y)$ be the M-polynomial of a graph G. Then one can calculate above TI from the M-polynomial with help of following relationships [18].

Table 1 Table of Topological index and derivation from $M(G; x, y)$ or $f(x, y)$.

Topological index	Notation	Derivation from f(x,y)
General Randic index	$R_\alpha(G)$	$\left(D_x^\alpha D_y^\alpha\right)\left(M(G; x, y)\right)\big\vert_{x=y=1}$
1st Zagreb	$M_1(G)$	$\left(D_x + D_y\right)\left(M(G; x, y)\right)\big\vert_{x=y=1}$
2nd Zagreb	$M_2(G)$	$\left(D_x D_y\right)\left(M(G; x, y)\right)\big\vert_{x=y=1}$
2nd modified Zagreb	$m_{M_2}(G)$	$\left(S_x S_y\right)\left(M(G; x, y)\right)\big\vert_{x=y=1}$
Augmented Zagreb	$A(G)$	$S_x^3 Q_{-2} J D_x^3 D_y^3\left(M(G; x, y)\right)\big\vert_{x=1}$
Harmonic index	$H(G)$	$2\, S_x J\left(M(G; x, y)\right)\big\vert_{x=1}$
Inverse Sum index	$I(G)$	$S_x J D_x D_y\left(M(G; x, y)\right)\big\vert_{x=1}$
Symmetric Division index	$SDD(G)$	$\left(D_x S_y + D_y S_x\right)\left(M(G; x, y)\right)\big\vert_{x=y=1}$

Where $D_x(f(x,y)) = x\frac{\partial(f(x,y))}{\partial x}$, $D_y(f(x,y)) = y\frac{\partial(f(x,y))}{\partial y}$, $S_x(f(x,y)) = \int_0^x \frac{f(t,y)}{t}dt$, $S_y(f(x,y)) = \int_0^y \frac{f(x,t)}{t}dt$, $J(f(x,y)) = f(x,x)$ and $Q_\alpha(f(x,y)) = x^\alpha f(x,y)$, $\alpha \neq 0$.

Molecular graph of TiO_2 crystal

Let G be the molecular graph of the crystallographic structure of $TiO_2[m,n,t]$ with $m \times n$ numbers of unit cells in the plane and t layers. In **Figures 3** and **4** we have shown the graph of $TiO_2[1,1,1]$ and $TiO_2[3,3,3]$ respectively. The cardinality of vertices and edges of the given molecular graph $TiO_2[m,n,t]$ are $(m+1)(n+1)(t+1) + 5mnt + 2mt$ and $10mnt + 2m(n+1)t + (m+1)\,n\,(t+1)$ respectively. The number of vertices of degree 2 is $8 + 4mt$, degree 3 is $4(m-1) + 2(n-1) + 4(t-1) + 2mt(2n-1)$, degree 4 is $2(n-1)$, degree 5 is $2(m-1)(n-1) + (t-1)(2m+2n-4)$, degree 6 is mnt and the number of vertices of degree 8 is $(m-1)(n-1)(t-1)$. The term degree means the number of bonding 1 atom has in the given system.

In the unit cell of TiO_2, the degree of the oxygen atom O_1, O_2, O_4, O_5 as shown in **Figure 1** is 2 but the actual degree of the these atoms in formation of the TiO_2 supercell as shown in **Figure 2** is 3. The missing 1 degree is shared with other unit cell. As a result the complete understanding of degree of these oxygen atoms is incomplete in case of a single unit cell.

Here the different relations such as vertices, edges, M-polynomials and TI are expressed in terms of m, n, t where $m > 1, n > 1, t > 1$ and are found to be invalid for $m = n = t = 1$. This means these definitions are not applicable for single unit cell.

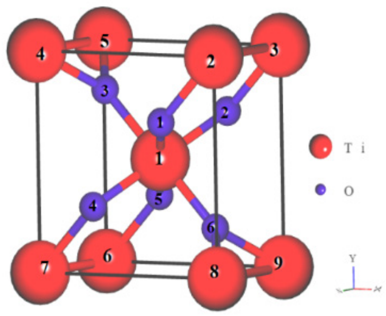

Figure 1 The unit cell of TiO_2.

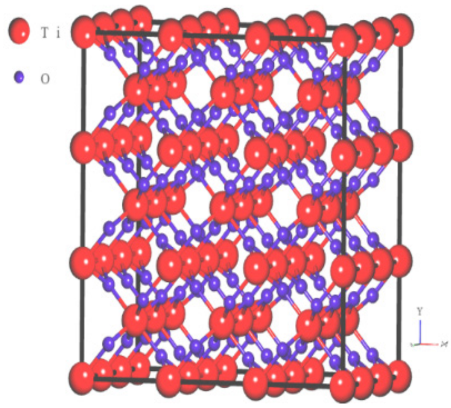

Figure 2 $TiO_2(3 \times 3 \times 3)$ supercell.

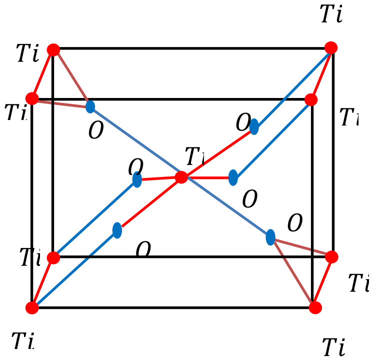

Figure 3 Unit cell of TiO_2.

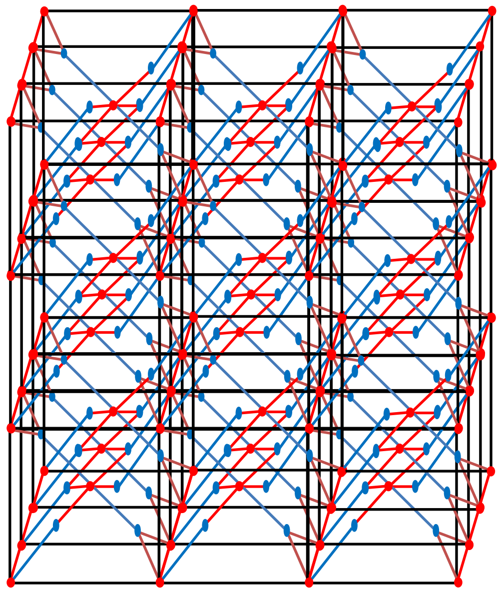

Figure 4 Molecular graph of crystallographic structure of TiO_2 [3,3,3].

The edge set of $TiO_2[m, n, t] \cong G(m, n, t)$ has the following fourteen partitions,

$E_1 = E_{\{2,2\}} = \{e = uv \in E(G) | d_u = 2, d_v = 2\}$
$E_2 = E_{\{2,3\}} = \{e = uv \in E(G) | d_u = 2, d_v = 3\}$
$E_3 = E_{\{2,4\}} = \{e = uv \in E(G) | d_u = 2, d_v = 4\}$
$E_4 = E_{\{2,5\}} = \{e = uv \in E(G) | d_u = 2, d_v = 5\}$
$E_5 = E_{\{2,6\}} = \{e = uv \in E(G) | d_u = 2, d_v = 6\}$
$E_6 = E_{\{3,3\}} = \{e = uv \in E(G) | d_u = 3, d_v = 3\}$
$E_7 = E_{\{3,4\}} = \{e = uv \in E(G) | d_u = 3, d_v = 4\}$
$E_8 = E_{\{3,5\}} = \{e = uv \in E(G) | d_u = 3, d_v = 5\}$
$E_9 = E_{\{3,6\}} = \{e = uv \in E(G) | d_u = 3, d_v = 6\}$
$E_{10} = E_{\{3,8\}} = \{e = uv \in E(G) | d_u = 3, d_v = 8\}$
$E_{11} = E_{\{4,4\}} = \{e = uv \in E(G) | d_u = 4, d_v = 4\}$
$E_{12} = E_{\{5,5\}} = \{e = uv \in E(G) | d_u = 5, d_v = 5\}$
$E_{13} = E_{\{5,8\}} = \{e = uv \in E(G) | d_u = 5, d_v = 8\}$
$E_{14} = E_{\{8,8\}} = \{e = uv \in E(G) | d_u = 8, d_v = 8\}$

such that

$|E_1(G)| = 4$, $|E_2(G)| = 4m + 4t$, $|E_3(G)| = 4$, $|E_4(G)| = 4mt - 4m - 4t + 4$,
$|E_5(G)| = 4mt$, $|E_6(G)| = 4m + 2n + 4t - 10$, $|E_7(G)| = 4n - 4$

$|E_8(G)| = 6mn + 4mt + 6nt - 6m - 12n - 6t + 8,$
$|E_9(G)| = 4mnt, |E_{10}(G)| = 6mnt - 6mn - 6mt - 6nt + 6m + 6n + 6t - 6$
$|E_{11}(G)| = 2n - 4, |E_{12}(G)| = 2mn + 2nt - 4m - 4n - 4t + 8$
$|E_{13}(G)| = 2mt - 2m - 2t + 2$
$|E_{14}(G)| = mnt - mn - 2mt - nt + 2m + n + 2t - 2.$

M-polynomial of TiO_2 [m, n, t]

Consider the graph $G(m,n,t)$ of TiO_2 with $m > 1, n > 1, t > 1$, then the M-polynomial of this graph is given by:

$$M(G;x,y) = f(x,y) = \sum_{i\le j} m_{ij}(G)x^i y^j$$

$$= \sum_{2\le 2} m_{22}(G)x^2y^2 + \sum_{2\le 3} m_{23}(G)x^2y^3 + \sum_{2\le 4} m_{24}(G)x^2y^4 + \sum_{2\le 5} m_{25}(G)x^2y^5 + \sum_{2\le 6} m_{26}(G)x^2y^6 + \sum_{3\le 3} m_{33}(G)x^3y^3 + \sum_{3\le 4} m_{34}(G)x^3y^4 + \sum_{3\le 5} m_{35}(G)x^3y^5 + \sum_{3\le 6} m_{36}(G)x^3y^6 + \sum_{3\le 8} m_{38}(G)x^3y^8 + \sum_{4\le 4} m_{44}(G)x^4y^4 + \sum_{5\le 5} m_{55}(G)x^5y^5 + \sum_{5\le 8} m_{58}(G)x^5y^8 + \sum_{8\le 8} m_{88}(G)x^8y^8$$

$$= |E_1|x^2y^2 + |E_2|x^2y^3 + |E_3|x^2y^4 + |E_4|x^2y^5 + |E_5|x^2y^6 + |E_6|x^3y^3 + |E_7|x^3y^4 + |E_8|x^3y^5 + |E_9|x^3y^6 + |E_{10}|x^3y^8 + |E_{11}|x^4y^4 + |E_{12}|x^5y^5 + |E_{13}|x^5y^8 + |E_{14}|x^8y^8$$

$$= 4x^2y^2 + 4(m+t)x^2y^3 + 4x^2y^4 + 4(mt - m - t + 1)x^2y^5 + (4mt)x^2y^6 + (4m + 2n + 4t - 10)x^3y^3 + 4(n-1)x^3y^4 + (6mn + 4mt + 6nt - 6m - 12n - 6t + 8)x^3y^5 + (4mnt)x^3y^6 + 6(mnt - mn - mt - nt + m + n + t - 1)x^3y^8 + 2(n-2)x^4y^4 + (2mn + 2nt - 4m - 4n - 4t + 8)x^5y^5 + 2(mt - m - t + 1)x^5y^8 + (mnt - mn - 2mt - nt + 2t + 2m + n - 2)x^8y^8$$

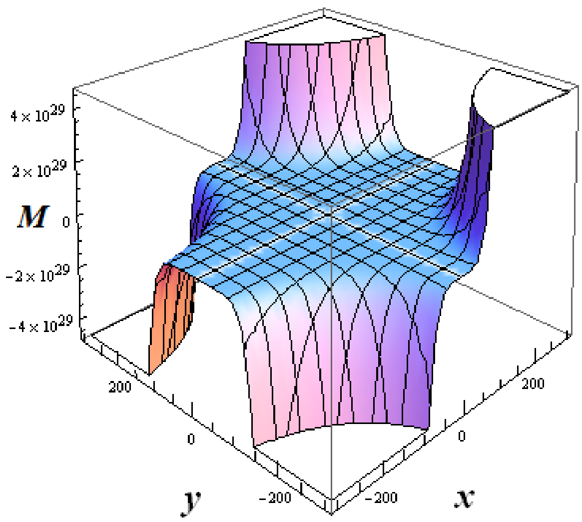

Figure 5 3D plot of M-polynomial of the TiO_2 crystal.

In **Figure 5**, we have plotted the 3D graphics of the M-polynomial keeping m, n, t fixed using Mathematica 9 software.

Computation of TI $G(m,n,t)$ from M-polynomial

Now we compute some degree-based TI of TiO_2 from the M-polynomial. Consider the Graph $G(m,n,t)$ of TiO_2 with $m > 1, n > 1, t > 1$;

The M-polynomial of the crystallographic structure $G(m,n,t) \cong TiO_2[m,n,t]$ is:

$$M(G(m,n,t);x,y) = 4x^2y^2 + 4(m+t)x^2y^3 + 4x^2y^4 + 4(mt-m-t+1)x^2y^5 + (4mt)x^2y^6 + (4m+2n+4t-10)x^3y^3 + 4(n-1)x^3y^4 + (6mn+4mt+6nt-6m-12n-6t+8)x^3y^5 + (4mnt)x^3y^6 + 6(mnt-mn-mt-nt+m+n+t-1)x^3y^8 + 2(n-2)x^4y^4 + (2mn+2nt-4m-4n-4t+8)x^5y^5 + 2(mt-m-t+1)x^5y^8 + (mnt-mn-2mt-nt+2m+2t+n-2)x^8y^8.$$

Now, we have the following computations:

$$D_xf(x,y) = x\frac{\partial f(x,y)}{\partial x}$$
$$= 8x^2y^2 + 8(m+t)x^2y^3 + 8x^2y^4 + 8(mt-m-t+1)x^2y^5 + 8mtx^2y^6 + 6(2m+n+2t-5)x^3y^3 + 12(n-1)x^3y^4 + 6(3mn+2mt+3nt-3m-6n-3t+4)x^3y^5 + 12mntx^3y^6 + 18(mnt-mn-mt-nt+m+n+t-1)x^3y^8 + 8(n-2)x^4y^4 + 10(mn+nt-2m-2n-2t+4)x^5y^5 + 10(mt-m-t+1)x^5y^8 + 8(mnt-mn-2mt-nt+2m+2t+n-2)x^8y^8.$$

$$D_yf(x,y) = y\frac{\partial f(x,y)}{\partial y}$$
$$= 8y^2 + 12(m+t)x^2y^3 + 16x^2y^4 + 20(mt-m-t+1)x^2y^5 + (24mt)x^2y^6 + 3(4m+2n+4t-10)x^3y^3 + 16(n-1)x^3y^4 + 5(6mn+4mt+6nt-6m-12n-6t+8)x^3y^5 + (24mnt)x^3y^6 + 48(mnt-mn-mt-nt+m+n+t-1)x^3y^8 + 8(n-2)x^4y^4 + 5(2mn+2nt-4m-4n-4t+8)x^5y^5 + 16(mt-m-t+1)x^5y^8 + 8(mnt-mn-2mt-nt+2m+2t+n-2)x^8y^8.$$

$$S_xf(x,y) = \int_0^x \frac{f(t,y)}{t}dt$$
$$= 2x^2y^2 + 2(m+t)x^2y^3 + 2x^2y^4 + 2(mt-m-t+1)x^2y^5 + 2mtx^2y^6 + \tfrac{2}{3}(2m+n+2t-5)x^3y^3 + \tfrac{4}{3}(n-1)x^3y^4 + \tfrac{2}{3}(3mn+2mt+3nt-3m-6n-3t+4)x^3y^5 + \tfrac{4}{3}mntx^3y^6 + 2(mnt-mn-mt-nt+m+n+t-1)x^3y^8 + \tfrac{1}{2}(n-2)x^4y^4 + \tfrac{2}{5}(mn+nt-2m-2n-2t+4)x^5y^5 + \tfrac{2}{5}(mt-m-t+1)x^5y^8 + \tfrac{1}{8}(mnt-mn-2mt-nt+2m+2t+n-2)x^8y^8.$$

$$S_yf(x,y) = \int_0^y \frac{f(x,t)}{t}dt$$
$$= 2x^2y^2 + \tfrac{4}{3}(m+t)x^2y^3 + x^2y^4 + \tfrac{4}{5}(mt-m-t+1)x^2y^5 + \tfrac{2}{3}mtx^2y^6 + \tfrac{2}{3}(2m+n+2t-5)x^3y^3 + (n-1)x^3y^4 + \tfrac{2}{5}(3mn+2mt+3nt-3m-6n-3t+4)x^3y^5 + \tfrac{2}{3}mntx^3y^6 + \tfrac{3}{4}(mnt-mn-mt-nt+m+n+t-1)x^3y^8 + \tfrac{1}{2}(n-2)x^4y^4 + \tfrac{2}{5}(mn+nt-2m-2n-2t+4)x^5y^5 + \tfrac{1}{4}(mt-m-t+1)x^5y^8 + \tfrac{1}{8}(mnt-mn-2mt-nt+2m+2t+n-2)x^8y^8.$$

$$D_xD_yf(x,y) = 16x^2y^2 + 24(m+t)x^2y^3 + 32x^2y^4 + 40(mt-m-t+1)x^2y^5 + 48mtx^2y^6 + 18(2m+n+2t-5)x^3y^3 + 48(n-1)x^3y^4 + 30(3mn+2mt+3nt-3m-6n-3t+4)x^3y^5 + 72mntx^3y^6 + 144(mnt-mn-mt-nt+m+n+t-1)x^3y^8 + 32(n-2)x^4y^4 + 50(mn+nt-2m-2n-2t+4)x^5y^5 + 80(mt-m-t+1)x^5y^8 + 64(mnt-mn-2mt-nt+2m+2t+n-2)x^8y^8.$$

$S_xS_yf(x,y) = x^2y^2 + \frac{2}{3}(m+t)x^2y^3 + \frac{1}{2}x^2y^4 + \frac{2}{5}(mt-m-t+1)x^2y^5 + \frac{1}{3}mtx^2y^6 + \frac{2}{9}(2m+n+2t-5)x^3y^3 + \frac{1}{3}(n-1)x^3y^4 + \frac{2}{15}(3mn+2mt+3nt-3m-6n-3t+4)x^3y^5 + \frac{2}{9}mntx^3y^6 + \frac{1}{4}(mnt-mn-mt-nt+m+n+t-1)x^3y^8 + \frac{1}{8}(n-2)x^4y^4 + \frac{2}{25}(mn+nt-2m-2n-2t+4)x^5y^5 + \frac{1}{20}(mt-m-t+1)x^5y^8 + \frac{1}{64}(mnt-mn-2mt-nt+2m+2t+n-2)x^8y^8.$

$D_yS_xf(x,y) = 4x^2y^2 + 6(m+t)x^2y^3 + 8x^2y^4 + 10(mt-m-t+1)x^2y^5 + 12mtx^2y^6 + 2(2m+n+2t-5)x^3y^3 + \frac{16}{3}(n-1)x^3y^4 + 5(3mn+2mt+3nt-3m-6n-3t+4)x^3y^5 + 8mntx^3y^6 + 16(mnt-mn-mt-nt+m+n+t-1)x^3y^8 + 2(n-2)x^4y^4 + 2(mn+nt-2m-2n-2t+4)x^5y^5 + \frac{16}{5}(mt-m-t+1)x^5y^8 + (mnt-mn-2mt-nt+2m+2t+n-2)x^8y^8.$

$D_xS_yf(x,y) = 4x^2y^2 + \frac{8}{3}(m+t)x^2y^3 + 2x^2y^4 + \frac{8}{5}(mt-m-t+1)x^2y^5 + \frac{4}{3}mtx^2y^6 + 2(2m+n+2t-5)x^3y^3 + 3(n-1)x^3y^4 + \frac{6}{5}(3mn+2mt+3nt-3m-6n-3t+4)x^3y^5 + 2mntx^3y^6 + \frac{9}{4}(mnt-mn-mt-nt+m+n+t-1)x^3y^8 + 2(n-2)x^4y^4 + 2(mn+nt-2m-2n-2t+4)x^5y^5 + \frac{5}{4}(mt-m-t+1)x^5y^8 + (mnt-mn-2mt-nt+2m+2t+n-2)x^8y^8.$

$D_x^{\alpha}D_y^{\alpha}f(x,y) = 2^{\alpha}.2^{\alpha}.4x^2y^2 + 2^{\alpha}.3^{\alpha}.4(m+t)x^2y^3 + 2^{\alpha}.4^{\alpha}.4x^2y^4 + 2^{\alpha}.5^{\alpha}.4(m-1)(t-1)x^2y^5 + 2^{\alpha}.6^{\alpha}.4mtx^2y^6 + 3^{\alpha}.3^{\alpha}.2(2m+n+2t-5)x^3y^3 + 3^{\alpha}.4^{\alpha}.4(n-1)x^3y^4 + 3^{\alpha}.5^{\alpha}.2(3mn+2mt+3nt-3m-6n-3t+4)x^3y^5 + 3^{\alpha}.6^{\alpha}.4mntx^3y^6 + 3^{\alpha}.8^{\alpha}.6(m-1)(n-1)(t-1)x^3y^8 + 4^{\alpha}.4^{\alpha}.2(n-2)x^4y^4 + 5^{\alpha}.5^{\alpha}.2(mn+nt-2m-2n-2t+4)x^5y^5 + 5^{\alpha}.8^{\alpha}.2(m-1)(t-1)x^5y^8 + 8^{\alpha}.8^{\alpha}(mnt-mn-2mt-nt+2m+2t+n-2)x^8y^8.$

$S_x^{\alpha}S_y^{\alpha}f(x,y) = \frac{4}{2^{\alpha}.2^{\alpha}}x^2y^2 + \frac{4}{2^{\alpha}.3^{\alpha}}(m+t)x^2y^3 + \frac{4}{2^{\alpha}.4^{\alpha}}x^2y^4 + \frac{4}{2^{\alpha}.5^{\alpha}}(m-1)(t-1)x^2y^5 + \frac{4}{2^{\alpha}.6^{\alpha}}mtx^2y^6 + \frac{2}{3^{\alpha}.3^{\alpha}}(2m+n+2t-5)x^3y^3 + \frac{4}{3^{\alpha}.4^{\alpha}}(n-1)x^3y^4 + \frac{2}{3^{\alpha}.5^{\alpha}}(3mn+2mt+3nt-3m-6n-3t+4)x^3y^5 + \frac{4}{3^{\alpha}.6^{\alpha}}mntx^3y^6 + \frac{6}{3^{\alpha}.8^{\alpha}}(mnt-mn-mt-nt+m+n+t-1)x^3y^8 + \frac{2}{4^{\alpha}.4^{\alpha}}(n-2)x^4y^4 + \frac{2}{5^{\alpha}.5^{\alpha}}(mn+nt-2m-2n-2t+4)x^5y^5 + \frac{2}{8^{\alpha}.8^{\alpha}}(m-1)(t-1)x^5y^8 + (mnt-mn-2mt-nt+2m+2t+n-2)x^8y^8.$

$S_xJf(x,y) = x^4 + \frac{4}{5}(m+t)x^5 + \frac{2}{3}x^6 + \frac{4}{7}(mt-m-t+1)x^7 + \frac{4}{8}mtx^8 + \frac{1}{3}(2m+n+2t-5)x^6 + \frac{4}{7}(n-1)x^7 + \frac{1}{4}(3mn+2mt+3nt-3m-6n-3t+4)x^8 + \frac{4}{9}mntx^9 + \frac{6}{11}(m-1)(n-1)(t-1)x^{11} + \frac{1}{4}(n-2)x^8 + \frac{1}{5}(mn+nt-2m-2n-2t+4)x^{10} + \frac{2}{13}(m-1)(t-1)x^{13} + \frac{1}{16}(mnt-mn-2mt-nt+2m+2t+n-2)x^{16}.$

$S_xJD_xD_yf(x,y) = 4x^4 + \frac{24}{5}(m+t)x^5 + \frac{8}{3}x^6 + \frac{40}{7}(m-1)(t-1)x^7 + 6mtx^8 + 3(2m+n+2t-5)x^6 + \frac{48}{7}(n-1)x^7 + \frac{15}{4}(3mn+2mt+3nt-3m-6n-3t+4)x^8 + 8mntx^9 + \frac{144}{11}(mnt-mn-mt-nt+m+n+t-1)x^{11} + 4(n-2)x^8 + 5(mn+nt-2m-2n-2t+4)x^{10} + \frac{80}{13}(m-1)(t-1)x^{13} + 4(mnt-mn-2mt-nt+2m+2t+n-2)x^{16}.$

$S_x^3Q_{-2}JD_x^3D_y^3f(x,y) = \frac{2^3.2^3.4}{2^3}x^2 + \frac{2^3.3^3}{3^3}4(m+t)x^3 + \frac{2^3.4^3.4}{4^3}x^4 + \frac{2^3.5^3}{5^3}4(m-1)(t-1)x^5 + \frac{2^3.6^3}{6^3}4mtx^6 + \frac{3^3.3^3}{4^3}2(2m+n+2t-5)x^4 + \frac{3^3.4^3}{5^3}4(n-1)x^5 + \frac{3^3.6^3}{7^3}4mntx^7 + \frac{3^3.8^3}{9^3}6(mnt-mn-mt-nt+m+n+t-1)x^9 + \frac{4^3.4^3}{6^3}2(n-2)x^6 + \frac{5^3.5^3}{8^3}2(mn+nt-m-2n-t+2)x^8 + \frac{5^3.8^3}{11^3}2(m-1)(t-1)x^{11} + \frac{8^3.8^3}{14^3}(mnt-mn-2mt-nt+2m+2t+n-2)x^{14}$

Using these values we get the TI defined in **Table 1** as follows:

1) $M_1(G) = 118mnt - 14mn + 20mt - 4nt + 2n + 20.$

2) $M_2(G) = 280mnt - 68mn - 44mt - 68nt + 22m + 26n + 22t + 14.$

3) $m_{M_2} = \frac{317}{576}mnt + \frac{343}{1600}mn + \frac{61}{96}mt + \frac{343}{1600}nt + \frac{2753}{7200}m - \frac{199}{14400}n + \frac{2753}{7200}t + \frac{7399}{7200}.$

4) $R_\alpha(G) = 2^\alpha.2^\alpha.4 + 2^\alpha.3^\alpha.4(m+t) + 2^\alpha.4^\alpha.4 + 2^\alpha.5^\alpha.4(m-1)(t-1) + 2^\alpha.6^\alpha.4mt + 3^\alpha.3^\alpha.2(2m+n+2t-5) + 3^\alpha.4^\alpha.4(n-1) + 3^\alpha.5^\alpha.2(3mn+2mt+3nt-3m-6n-3t+4) + 3^\alpha.6^\alpha.4mnt + 3^\alpha.8^\alpha.6(mnt-mn-mt-nt+m+n+t-1) + 4^\alpha.4^\alpha.2(n-2) + 5^\alpha.5^\alpha.2(mn+nt-2m-2n-2t+4) + 5^\alpha.8^\alpha.2(m-1)(t-1) + 8^\alpha.8^\alpha(mnt-mn-2mt-nt+2m+2t+n-2).$

5) $RR_\alpha(G) = \frac{4}{2^\alpha.2^\alpha} + \frac{4}{2^\alpha.3^\alpha}(m+t) + \frac{4}{2^\alpha.4^\alpha} + \frac{4}{2^\alpha.5^\alpha}(m-1)(t-1) + \frac{4}{2^\alpha.6^\alpha}mt + \frac{2}{3^\alpha.3^\alpha}(2m+n+2t-5) + \frac{4}{3^\alpha.4^\alpha}(n-1) + \frac{2}{3^\alpha.5^\alpha}(3mn+2mt+3nt-3m-6n-3t+4) + \frac{4}{3^\alpha.6^\alpha}mnt + \frac{6}{3^\alpha.8^\alpha}(m-1)(n-1)(t-1) + \frac{2}{4^\alpha.4^\alpha}(n-2) + \frac{2}{5^\alpha.5^\alpha}(mn+nt-m-2n-t+2) + \frac{2}{5^\alpha.8^\alpha}(m-1)(t-1) + \frac{1}{8^\alpha.8^\alpha}(mnt-mn-2mt-nt+2m+2t+n-2).$

6) $I(G) = 4 + \frac{24}{5}(m+t) + \frac{16}{3} + \frac{40}{7}(m-1)(t-1) + 6mt + 3(2m+n+2t-5) + \frac{48}{7}(n-1) + \frac{15}{4}(3mn+2mt+3nt-3m-6n-3t+4) + 8mnt + \frac{144}{11}(mnt-mn-mt-nt+m+n+t-1) + 4(n-2) + 5(mn+nt-2m-2n-2t+4) + \frac{80}{13}(mt-m-t+1) + 4(mnt-mn-2mt-nt+2m+2t+n-2).$

7) $A(G) = \frac{2^3.2^3.4}{2^3} + \frac{2^3.3^3}{3^3}4(m+t) + \frac{2^3.4^3.4}{4^3} + \frac{2^3.5^3}{5^3}4(mt-m-t+1) + \frac{2^3.6^3}{6^3}4mt + \frac{3^3.3^3}{4^3}2(2m+n+2t-5) + \frac{3^3.4^3}{5^3}4(n-1) + \frac{3^3.6^3}{7^3}4mnt + \frac{3^3.8^3}{9^3}6(mnt-mn-mt-nt+m+n+t-1) + \frac{4^3.4^3}{6^3}2(n-2) + \frac{5^3.5^3}{8^3}2(mn+nt-2m-2n-2t+4) + \frac{5^3.8^3}{11^3}(2mt-m-t+1) + \frac{8^3.8^3}{14^3}(mnt-mn-2mt-nt+2m+2t+n-2).$

8) $H(G) = 2 + \frac{8}{5}(m+t) + \frac{4}{3} + \frac{8}{7}(mt-m-t+1) + mt + \frac{2}{3}(2m+n+2t-5) + \frac{8}{7}(n-1) + \frac{1}{2}(3mn+2mt+3nt-3m-6n-3t+4) + \frac{2.4}{9}mnt + \frac{2.6}{11}(mnt-mn-mt-nt+m+n+t-1) + \frac{2.2}{8}(n-2) + \frac{2.2}{10}(mn+nt-2m-2n-2t+4) + \frac{2.2}{13}(mt-m-t+1) + \frac{1.2}{16}(mnt-mn-2mt-nt+2m+2t+n-2).$

9) $SDD(G) = \frac{121}{4}mnt + \frac{219}{20}mn + \frac{134}{15}mt - \frac{53}{20}nt + \frac{19}{15}m + \frac{323}{9}n + \frac{139}{15}t + \frac{108}{5}.$

Discussion

Figures 6 - 8 show the variation of different TI with m, n, and t respectively. All the variations follow a straight line equation having different slopes. The plot for A(G) is overlapped with M_2. TI maintain the order of slope in all the figures i.e. A(G) = M_2 > M_1 > SDD > I(G) > Randic > H(G) > mM_2. Though a distinct difference can be observed in **Figure 7** where the slope of H(G) becomes nearly equal to Randic. This behavior of H(G) vs n can be ascribed to the degree of oxygen atoms in 3D crystal TiO_2. Revisiting the molecular graph section of TiO_2, these oxygen atoms (or points in molecule graph) carry the same degree if we increase m and t but when we replicate the unit cell along with n then the degree of oxygen (O1, O2, O4, O5) changes from 2 to 3. So, the variation of m and t (together and independently) does not bring any structural changes in terms of the degree of atoms compared to single unit cell. Whereas the variation of n brings a change in structure in terms of degrees of atoms compared to the unit cell. This further indicates that the topological index H(G) is linked to the total number of bonding in the system. So, this anisotropic behavior of the bonding pattern of oxygen atoms along n can be understood with the help of H(G). Similarly, all the other indices can also be linked to different physical properties which we'll investigate in the future.

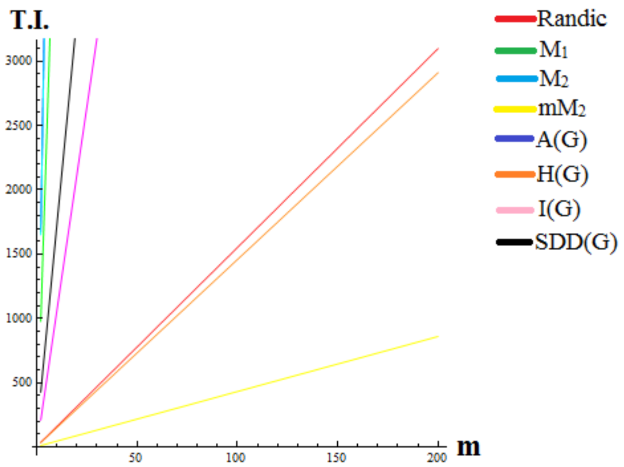

Figure 6 Plot of different TI vs m.

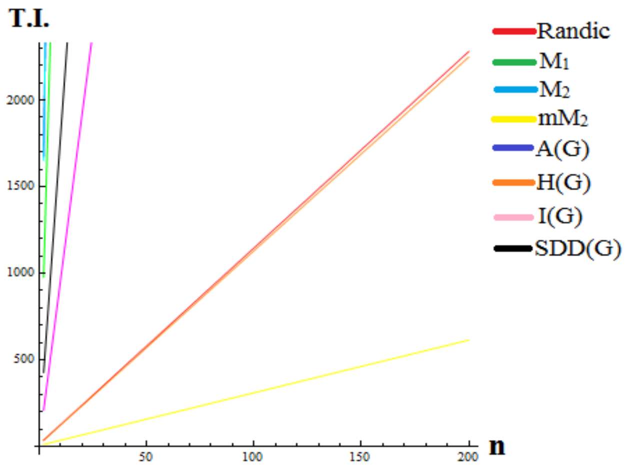

Figure 7 Plot of different TI vs n.

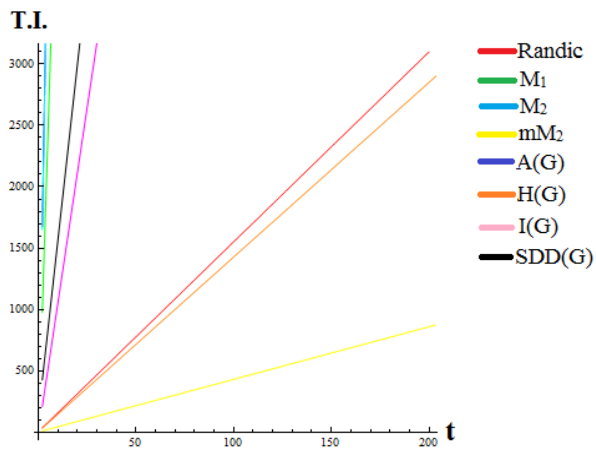

Figure 8 Plot of different TI vs t.

Conclusions

We have constructed M-polynomial for 3D TiO_2 crystal with the help of a molecular graph. During the study of the molecular graph we observed that the degree (bonds) of few oxygen atoms is not uniform with the extension of TiO_2 along 3D. This gives a new insight into the TiO_2 crystal. Further, we have calculated different TI with the help of M-polynomials. The variation of these indices along 3D is also studied. In the end we found that Harmonic index H(G) can be linked to the degree variation of oxygen atoms. Thus, we believe that these topological indices can be used as the benchmark for the study of different physical properties of TiO_2 crystals.

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