Hosoya Polynomials Of Some Semiconducotors

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Abstract

The Hosoya polynomial of a graph *G* is a graphical invariant polynomial that its first derivative at x = 1 is equal to the Wiener index and second derivative at x =1 is equal to the hyper–Wiener index. In this paper we compute the Hosoya polynomial of some semiconducotors [Caesium Chloride, Perovskite structure, Zinc blende structure, Rock-salt(Nacl)structure, Wurtzite structure, Chalcopyrite structure], Wiener index and hyper-Wiener index for then.

Keywords: Hosoya polynomial , graph

INTRODUCTION

The graph polynomial which we study in this paper was invented in 1988 by Hosoya [6](and was originally named the Wiener polynomial). We nevertheless call it the Hosoya polynomial. It is defined as follows. Let G be a connected graph on n vertices. The vertex and edge sets of G are $V(G) = \{x_1, x_2, \dots , x_n\}$ and $E(G) = \{y_1; y_2,\dots, y_m\}$, respectively. The length(= number of edges) of a shortest path between the vertices x_i, $x_j \in V(G)$ is their distance and is denoted by $d(x_i, x_j |G)$.

The number of (unordered) pairs of vertices of G, whose distance is k, is denoted by d(G, k).

Let D be the diameter of the graph G. Clearly, d(G, k) = 0 whenever k >D. Furthermore, d(G, k) > 0 for all k = 1,…, D . The Hosoya polynomial of G is

$$H(G, x)=\sum_{k=0}^{D} d(G, k)x^k.$$

The Hosoya polynomial has many chemical applications[4,1], especially two well-known Topological indices, i:e; Wiener index and hyper-Wiener index, can be directly obtained from this polynomial The Wiener index of a connected graph G, [2]W(G) is equal to the first derivative of the Hosoya polynomial at x=1

$$W(G) = H'(G, x)|_{x=1}.$$

The hyper-Wiener index of graph G, [1] WW(G) is the second derivative of the Hosoya polynomial at x=1

$$WW(G) = \frac{1}{2}(xH(G,\ x)''|x = 1).$$

[3]The semiconducotors is a part of a new graph and it is economically most important. Product founded an the basis of semiconducotor dvices such as computers(CPUs, Memories), optical storage media (CD, DVD). In this paper we would like to investigate the mathematical properties of some semiconducotors. we study the Hosoya Polynomial, Wiener index and hyper-Wiener index of some semiconducotors.

2. Hosoya Polynomials, Wiener Index and hyper-Wiener Index of Caesium chloride (CsCl) structure

[5]In section we calculate Hosoya Polynomials, Wiener Index and hyper-Wiener Index of Caesium chloride (CsCl) structure, Caesium chloride as a chemical compound is an ionic compound with the formula CsCl, representing equal proportions of Caesium and chloride and it is used chemicals production.

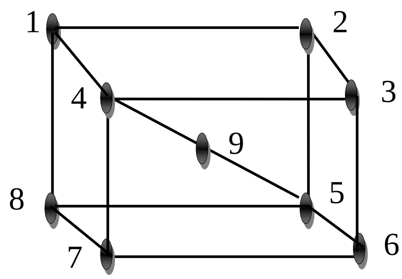

Figure 1. Caesium chloride

We calculate distance [path shortest] for all vertice with other vertices and eccentricity for all vertices by the following table. The eccentricity e(v) of a vertex v is the maximum distance from v to any other vertex.

d	1	2	3	4	5	6	7	8	9	e(v)
1	0	1	2	1	2	3	2	1	2	3
2	1	0	1	2	1	2	3	2	2	3
3	2	1	0	1	2	1	2	3	2	3
4	1	2	1	0	2	2	1	2	1	2
5	2	1	2	2	0	1	2	1	1	2
6	3	2	1	2	1	0	1	2	2	3
7	2	3	2	1	2	1	0	1	2	3
8	1	2	3	2	1	2	1	0	2	3
9	2	2	2	1	1	2	2	2	0	2

Table1.The number of pair vertices of struture CsCl that are at distance k of each other

Diameter (G) = 3

The Hosoya polynomial

is $H(G,x) = \sum_{k=0}^{3} d(G,k)x^k$

$= 9 + 14x + 19x^2 + 3x^3$

To find the Wiener index, we have

$W(G) = H'(G, x)|_{x=1}$

$H'(G, x) = 14 + 38x + 9x^2$.

$W(G) = H'(G, x)|_{x=1} = 14 + 38 + 9 = 61$

To find the hyper-Wiener index is

$WW(G) = \frac{1}{2}(xH(G,x))''|_{x=1}$

Now, $xH(G, x) = 9x + 14x^2 + 19x^3 + 3x^4$.

Then $(xH(G, x))' = 9 + 28x + 57x^2 + 12x^3$

$(xH(G , x))'' = 28 + 114x + 36x^2$

$WW(G) = \frac{1}{2}(28+114+36) = 89$.

3. Hosoya Polynomials, Wiener Index and hyper-Wiener Index of Zincblende Structure

[3]It is form of forms the Zinc sufide structure and it has cubic structure. It are used in electrical circuits, photodetectors, solar cells light-emitting, diodes and lasers are treated.

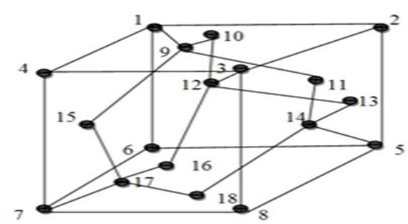

Figure 2. Zincblende structrue

We calculate distance [path shortest] for all vertice with other vertices and eccentricity for all vertices by the following table.

d	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	e(v)
1	0	1	2	1	2	1	2	3	1	2	2	3	4	3	2	4	3	4	4
2	1	0	1	2	1	2	2	2	2	3	3	2	3	2	3	3	4	5	5
3	2	1	0	1	2	3	2	1	3	2	4	1	2	3	4	2	3	4	4
4	1	2	1	0	3	2	1	2	2	3	3	2	3	4	3	3	2	3	4
5	2	1	2	3	0	1	2	1	3	4	2	3	2	1	4	4	3	2	4
6	1	2	3	2	1	0	1	2	2	3	3	4	3	2	3	3	2	3	4
7	2	3	2	1	2	1	0	1	3	4	4	3	4	3	2	2	1	2	4
8	3	2	1	2	1	2	1	0	4	3	3	2	3	2	3	3	2	3	4
9	1	2	3	2	3	2	3	4	0	1	1	2	3	2	1	3	2	3	4
10	2	3	2	3	4	3	4	3	1	0	2	1	2	3	2	2	3	4	4
11	2	3	4	3	2	3	4	3	1	2	0	3	2	1	2	4	3	2	4
12	3	2	1	2	3	4	3	2	2	1	3	0	1	2	3	1	2	3	4
13	4	3	2	3	2	3	4	3	3	2	2	1	0	1	4	2	3	2	4
14	3	2	3	4	1	2	3	2	2	3	1	2	1	0	3	3	2	1	4
15	2	3	4	3	4	3	2	3	1	2	2	3	4	3	0	2	1	2	4
16	4	3	2	3	4	3	2	3	3	2	4	1	2	3	2	0	1	2	4
17	3	4	3	2	3	2	1	2	2	3	3	2	3	2	1	1	0	1	4
18	4	5	4	3	2	3	2	3	3	4	2	3	2	1	2	2	1	0	5

Table 2. The number of pair vertices of Zincblende structure that are at distance k of each other

Diameter (G) = 5

The Hosoya polynomial is

$$H(G,x) = \sum_{k=0}^{5} d(G,k)x^k$$

$= 18 + 28x + 54x^2 + 51x^3 + 19x^4 + x^5$

To find the Wiener index of G, we have

$W(G) = H'(G, x)|_{x=1}$

$H'(G, x) = 28 + 110x + 153x^2 + 76x^3 + 5x^4$

$W(G) = H'(G, x)|_{x=1} = 28 + 110 + 153 + 76 + 5$

$= 372$

To calculate the hyper-Wiener index is

$$WW(G) = \frac{1}{2}(xH(G,x))''|_{x=1}$$

Now, $xH(G, x) = 18x + 28x^2 + 55x^3 + 51x^4 + 19x^5 + x^6$.

Then $(xH(G, x))' = 18 + 56x + 165x^2 + 204x^3 + 95x^4 + 6x^5$

$(xH(G, x))'' = 56 + 330x + 612x^2 + 380x^3 + 30x^4$

$$WW(G) = \frac{1}{2}(56 + 330 + 612 + 380 + 30)$$

$= 704.$

4. Hosoya Polynomials, Wiener Index and hyper-Wiener Index of Perovskite structure ($BaTiO_3$) a Cell with 12-Fold (cuboctahedrally) configured Ba

[7]The Perovskite family includes many titanates used in various electroceramic applications, for example, electronic, electro-optical, and electromechanical applications of ceramics. Barium titanate, Perovskite structure, is a common ferroelectric material with a high dielectric constant, widely utilized to manufacture electronic components such as mutilayer capacitors (MLCs), PTC thermistors, piezoelectric transducers, and a variety of electro-optic devices.

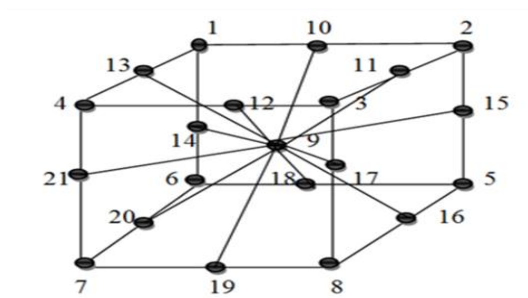

Figure 3. Perovskite structure ($BaTiO_3$) a cell with 12-fold (cuboctahedrally) configured Ba

Table 3. The number of pair vertices of Perovskite structure ($BaTiO_3$) a cell with 12-fold (cuboctahedrally) configured Ba that are at

d	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	e(v)
1	0	2	4	2	4	2	4	4	2	1	3	3	1	1	3	3	3	3	3	3	3	4
2	2	0	2	4	2	4	4	4	2	1	1	3	3	3	1	3	3	3	3	3	3	4
3	4	2	0	2	4	4	4	2	2	3	1	1	3	3	3	3	1	3	3	3	3	4
4	2	4	2	0	4	4	2	4	2	3	3	1	1	3	3	3	3	3	3	3	1	4
5	4	2	4	4	0	2	4	2	2	3	3	3	3	3	1	1	3	1	3	3	3	4
6	2	4	4	4	2	0	2	4	2	3	3	3	3	1	3	3	3	1	3	1	3	4
7	4	4	4	2	4	2	0	2	2	3	3	3	3	3	3	3	3	3	1	1	1	4
8	4	4	2	4	2	4	2	0	2	3	3	3	3	3	3	1	1	3	1	3	3	4
9	2	2	2	2	2	2	2	2	0	1	1	1	1	1	1	1	1	1	1	1	1	2
10	1	1	3	3	3	3	3	3	1	0	2	2	2	2	2	2	2	2	2	2	2	3
11	3	1	1	3	3	3	3	3	1	2	0	2	2	2	2	2	2	2	2	2	2	3
12	3	3	1	1	3	3	3	3	1	2	2	0	2	2	2	2	2	2	2	2	2	3
13	1	3	3	1	3	3	3	3	1	2	2	2	0	2	2	2	2	2	2	2	2	3
14	1	3	3	3	3	1	3	3	1	2	2	2	2	0	2	2	2	2	2	2	2	3
15	3	1	3	3	1	3	3	3	1	2	2	2	2	2	0	2	2	2	2	2	2	3
16	3	3	3	3	1	3	3	1	1	2	2	2	2	2	2	0	2	2	2	2	2	3
17	3	3	1	3	3	3	3	1	1	2	2	2	2	2	2	2	0	2	2	2	2	3
18	3	3	3	3	1	1	3	3	1	2	2	2	2	2	2	2	2	0	2	2	2	3
19	3	3	3	3	3	3	1	1	1	2	2	2	2	2	2	2	2	2	0	2	2	3
20	3	3	3	3	3	1	1	3	1	2	2	2	2	2	2	2	2	2	2	0	2	3
21	3	3	3	1	3	3	1	3	1	2	2	2	2	2	2	2	2	2	2	2	0	3

Diameter (G) = 4

The Hosoya polynomial is

$H(G,x) = \sum_{k=0}^{4} d(G,k)x^k = 21 + 36x + 86x^2 + 72x^3 + 16x^4$

To find Wiener index of G , we have $W(G) = H'(G, x)|_{x=1}$

$H'(G, x) = 36 + 172x + 216x^2 + 64x^3$

$W(G) = H'(G, x)|_{x=1} = 36 + 172 + 216 + 64$
$= 488$

To calculate the hyper-Wiener index is

$WW(G) = \frac{1}{2}(xH(G,x))''|_{x=1}$

Now, $xH(G, x) = 21x + 36x^2 + 86x^3 + 72x^4 + 16x^5$. Then $(xH(G, x))' = 21 + 72x + 258x^2 + 288x^3 + 80x^4$

$(xH(G,x))'' = 72 + 516x + 864x^2 + 320x^3$

$WW(G) = \frac{1}{2}(72 + 516 + 864 + 320) = 886.$

5. Hosoya Polynomials, Wiener Index and hyper-Wiener Index of Rocksalt (Nacl) structure

[3]As a chemical compound is an ionic compound with the formula NaCl, representing equal proportions of sodium and chloride and it is used Chemicals production, Chlor-alkali industry, Soda ash industry, Food industry, medicine and agriculture, Firefighting and Cleanser.

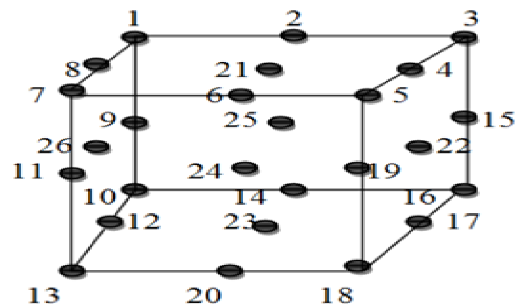

Figure 4. Rocksalt (Nacl) structure

We calculate distance [path shortest] for all vertice with other vertices and eccentricity for all vertices by the following table.

d	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	e(v)
1	0	1	2	3	4	3	2	1	1	2	3	3	4	3	3	4	5	6	5	5	0	0	0	0	0	0	6
2	1	0	1	2	3	4	3	2	2	3	4	4	5	4	2	3	4	5	4	6	0	0	0	0	0	0	6
3	2	1	0	1	2	3	4	3	3	4	5	5	6	3	1	2	3	4	3	5	0	0	0	0	0	0	6
4	3	2	1	0	1	2	3	4	4	5	4	6	5	4	2	3	4	3	2	4	0	0	0	0	0	0	6
5	4	3	2	1	0	1	2	3	5	6	3	5	4	5	3	4	3	2	1	3	0	0	0	0	0	0	6
6	3	4	3	2	1	0	1	2	4	5	2	4	3	6	4	5	4	3	2	4	0	0	0	0	0	0	6
7	2	3	4	3	2	1	0	1	3	4	1	3	2	5	5	6	5	4	3	3	0	0	0	0	0	0	6
8	1	2	3	4	3	2	1	0	2	3	2	4	3	4	4	5	6	5	4	4	0	0	0	0	0	0	6
9	1	2	3	4	5	4	3	2	0	1	4	2	3	2	4	3	4	5	6	4	0	0	0	0	0	0	6
10	2	3	4	5	6	5	4	3	1	0	3	1	2	1	3	2	3	4	5	3	0	0	0	0	0	0	6
11	3	4	5	4	3	2	1	2	4	3	0	2	1	4	6	5	4	3	4	2	0	0	0	0	0	0	6
12	3	4	5	6	5	4	3	4	2	1	2	0	1	2	4	3	4	3	4	2	0	0	0	0	0	0	6
13	4	5	6	5	4	3	2	3	3	2	1	1	0	3	5	4	3	2	3	1	0	0	0	0	0	0	6
14	3	4	3	4	5	6	5	4	2	1	4	2	3	0	2	1	2	3	4	4	0	0	0	0	0	0	6
15	3	2	1	2	3	4	5	4	4	3	6	4	5	2	0	1	2	3	4	4	0	0	0	0	0	0	6
16	4	3	2	3	4	5	6	5	3	2	5	3	4	1	1	0	1	2	3	3	0	0	0	0	0	0	6
17	5	4	3	4	3	4	5	6	4	3	4	4	3	2	2	1	0	1	2	2	0	0	0	0	0	0	6
18	6	5	4	3	2	3	4	5	5	4	3	3	2	3	3	2	1	0	1	1	0	0	0	0	0	0	6
19	5	4	3	2	1	2	3	4	6	5	4	4	3	4	4	3	2	1	0	2	0	0	0	0	0	0	6
20	5	6	5	4	3	4	3	4	4	3	2	2	1	4	4	3	2	1	2	0	0	0	0	0	0	0	6
21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
23	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
26	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Table 4. The number of pair vertices of Rocksalt (Nacl) structure that are at distance k of each other

Diameter (G) = 6

The Hosoya polynomial is

$H(G,x) = \sum_{k=0}^{6} d(G,k)x^k$

$= 26 + 24x + 36x^2 + 48x^3 + 48x^4 + 24x^5 + 10x^6$

To find the Wiener index, we have

$W(G) = H'(G, x)|_{x=1}$

$H'(G, x) = 24 + 72x + 144x^2 + 192x^3 + 120x^4 + 60x^5$

$W(G) = H'(G, x)|_{x=1} = 24 + 72 + 144 + 192 + 120 + 60 = 612$

To calculate the hyper-Wiener index is

$WW(G) = \frac{1}{2}(xH(G,x))''|_{x=1}$

Now, $xH(G, x) = 26x + 24x^2 + 36x^3 + 48x^4 + 48x^5 + 24x^6 + 10x^7$

Then $(xH(G, x))' = 26 + 48x + 108x^2 + 192x^3 + 240x^4 + 144x^5 + 70x^6$

$(xH(G, x))'' = 48 + 216x + 576x^2 + 960x^3 + 720x^4 + 420x^5$

$WW(G) = \frac{1}{2}(48 + 216 + 576 + 960 + 720 + 420)$

$= 1470.$

6. Hosoya Polynomials, Wiener index and hyper-Wiener index of wurtzite structure

[3] It is form of forms the Zinc sufide structure and it has hexagonal structure. It are used in electrical circuits, photodetectors, solar cells light-emitting, diodes and lasers are treated.

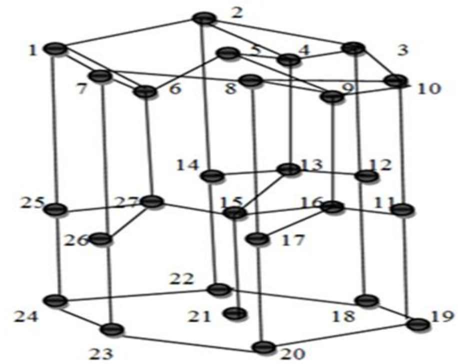

Figure 5. Wurtzite structrue

We find distance [path shortest] for all vertice with other vertices, dimeter and eccentricity for all vertices by the following table.

d	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	e(v)
1	0	1	2	2	2	1	1	2	3	3	4	3	3	2	3	4	3	4	5	4	4	3	3	2	1	2	2	5
2	1	0	1	1	2	2	2	3	3	2	3	2	2	1	3	4	4	3	4	5	4	2	4	3	2	3	3	5
3	2	1	0	1	2	3	3	2	2	1	2	1	2	2	3	3	3	2	3	4	4	3	5	4	3	4	4	5
4	2	1	1	0	1	2	3	3	2	2	3	2	1	2	2	3	4	3	4	5	3	3	5	4	3	4	3	5
5	2	2	2	1	0	1	2	2	1	2	3	3	2	3	3	2	3	4	4	4	4	4	4	4	3	3	2	4
6	1	2	3	2	1	0	1	2	2	3	4	4	3	3	2	3	3	5	5	4	3	4	3	3	2	2	3	5
7	1	2	3	3	2	1	0	1	2	2	3	4	4	3	3	3	2	5	4	3	4	4	2	3	2	1	2	5
8	2	3	2	3	2	2	1	0	1	1	2	5	4	4	3	2	1	4	3	2	4	5	3	4	3	2	3	5
9	3	3	2	2	1	2	2	1	0	1	2	4	3	4	2	1	2	4	3	3	3	5	4	5	4	3	3	5
10	3	2	1	2	2	3	2	1	1	0	1	2	3	3	3	2	2	3	2	3	4	4	4	5	4	3	4	5
11	4	3	2	3	3	4	3	2	2	1	0	3	3	4	2	1	2	2	1	2	3	3	3	4	4	4	3	4
12	3	2	1	2	3	4	4	5	4	2	3	0	1	2	2	3	4	1	2	3	3	2	4	3	4	4	3	5
13	3	2	2	1	2	3	4	4	3	3	3	1	0	1	1	2	3	2	3	4	2	2	4	3	3	3	2	4
14	2	1	2	2	3	3	3	4	4	3	4	2	1	0	2	3	4	2	3	4	3	1	3	2	3	4	3	4
15	3	3	3	2	3	2	3	3	2	3	2	2	1	2	0	1	2	3	3	3	1	3	3	3	2	2	1	3
16	4	4	3	3	2	3	3	2	1	2	1	3	2	3	1	0	1	3	2	2	2	4	3	4	3	3	2	4
17	3	4	3	4	3	3	2	1	2	2	2	4	3	4	2	1	0	3	2	1	3	4	2	3	4	3	3	4
18	4	3	2	3	4	5	5	4	4	3	2	1	2	2	3	3	3	0	1	2	4	1	3	2	3	4	4	5
19	5	4	3	4	4	5	4	3	3	2	1	2	3	3	3	2	2	1	0	1	4	2	2	3	4	3	4	5
20	4	5	4	5	4	4	3	2	3	3	2	3	4	4	3	2	1	2	1	0	4	3	1	2	3	2	3	5
21	4	4	4	3	4	3	4	4	3	4	3	3	2	3	1	2	3	4	4	4	0	4	4	4	3	3	2	4
22	3	2	3	3	4	4	4	5	5	4	3	2	2	1	3	4	4	1	2	3	4	0	2	1	2	3	3	5
23	3	4	5	5	4	3	2	3	4	4	3	4	4	3	3	3	2	3	2	1	4	2	0	1	2	1	2	5
24	2	3	4	4	4	3	3	4	5	5	4	3	3	2	3	4	3	2	3	2	4	1	1	0	1	2	2	5
25	1	2	3	3	3	2	2	3	4	4	4	4	3	3	2	3	4	3	4	3	3	2	2	1	0	2	1	4
26	2	3	4	4	3	2	1	2	3	3	4	4	3	4	2	3	3	4	3	2	3	3	1	2	2	0	1	4
27	2	3	4	3	2	1	2	3	3	4	3	3	2	3	1	2	3	4	4	3	2	3	2	2	1	1	0	4

Table 5. The number of pair vertices of wurtzite structure that are at distance k of each other

$$W(G) = H'(G, x)|_{x=1} = 46 + 192 + 357 + 231 + 65 = 891$$

To calculate the hyper-Wiener index is

$$WW(G) = \frac{1}{2}(xH(G,x))''|_{x=1}$$

Now, $xH(G, x) = 27x + 46x^2 + 96x^3 + 119x^4 + 77x^5 + 13x^6$.

Then $(xH(G, x))' = 27 + 92x + 288x^2 + 476x^3 + 385x^4 + 78x^5$

$(xH(G, x))'' = 92 + 576x + 1428x^2 + 1540x^3 + 390x^4$

$$WW(G) = \frac{1}{2}(92 + 576 + 1428 + 1540 + 390)$$
$$= 2013.$$

7. Hosoya Polynomials, Wiener Index and hyper-Wiener Index of Chalcopyrite Structure

[3]The chalcopyrite structure, named after the mineral chalcopyrite $CuFeS_2$ and also adopted by a number of $I - III - V\ I_2$ and $II - IV - V_2$ compounds, It is uses in.

1. They have potential optoelectronic applications as solar energy converters, nonlinear optical (NLO) devices, light emitting diodes (LED), and detectors.
2. They are useful for nonlinear optical frequency conversion applications.
3. It has application in photo- voltaic device.

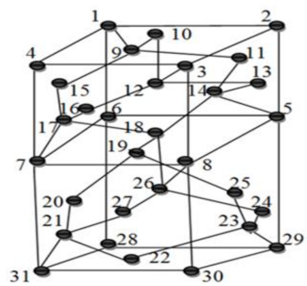

Figure 6. Chalcopyrite structrue

We find distance [path shortest] for all vertice with other vertices ,dimeter and eccentricity for all vertices by the following table.

d	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	e(v)
1	0	1	2	1	2	1	2	3	1	2	2	3	4	3	2	4	3	4	2	3	4	5	4	5	3	4	5	2	3	4	3	5
2	1	0	1	2	1	2	3	2	2	3	3	2	3	2	3	3	4	3	3	5	5	4	3	4	4	3	4	3	2	3	4	5
3	2	1	0	1	2	3	2	1	3	2	4	1	2	3	4	2	3	3	4	5	4	5	4	3	5	2	3	4	3	2	3	5
4	1	2	1	0	3	2	1	2	2	3	3	2	3	4	3	3	2	3	3	4	3	4	5	4	4	3	4	3	4	3	2	5
5	2	1	2	3	0	1	2	1	3	4	2	3	2	1	4	4	3	2	2	4	4	3	2	3	3	2	3	2	1	2	3	4
6	1	2	3	2	1	0	1	2	2	3	3	4	3	2	3	3	2	2	1	2	3	4	3	4	2	3	4	1	2	3	2	4
7	2	3	2	1	2	1	0	1	3	4	4	3	4	3	2	2	1	2	2	3	2	3	4	3	3	2	3	2	3	2	1	4
8	3	2	1	2	1	2	1	0	4	3	3	2	3	2	3	3	2	2	3	4	3	4	3	2	4	1	2	3	2	1	2	4
9	1	2	3	2	3	2	3	4	0	1	1	2	3	2	1	3	2	3	3	4	5	6	5	5	4	4	5	3	4	5	4	6
10	2	3	2	3	4	3	4	3	1	0	2	1	2	3	2	2	3	4	4	5	6	7	6	6	5	4	6	4	5	4	5	7
11	2	3	4	3	2	3	4	3	1	2	0	3	2	1	2	4	3	2	3	4	5	5	4	4	4	3	4	4	3	4	5	5
12	3	2	1	2	3	4	3	2	2	1	3	0	1	2	3	1	2	3	4	5	5	6	5	5	5	3	5	5	4	3	4	6
13	4	3	2	3	2	3	4	3	3	2	2	1	0	1	4	2	3	2	3	4	5	5	4	4	4	3	4	4	3	4	5	5
14	3	2	3	4	1	2	3	2	2	3	1	2	1	0	3	3	2	1	2	3	4	4	3	3	3	2	3	3	2	3	4	4
15	2	3	4	3	4	3	2	3	1	2	2	3	4	3	0	2	1	2	3	4	4	5	5	4	4	3	4	4	5	4	3	5
16	4	3	2	3	4	3	2	3	3	2	4	1	2	3	2	0	1	2	3	4	4	5	5	4	4	3	4	4	5	4	3	5
17	3	4	3	2	3	2	1	2	2	3	3	2	3	2	1	1	0	1	2	3	3	4	4	3	3	2	3	3	4	3	2	4
18	4	3	3	3	2	2	2	2	3	4	2	3	2	1	2	2	1	0	1	2	3	4	3	2	2	1	2	3	4	3	3	4
19	2	3	4	3	2	1	2	3	3	4	3	4	3	2	3	3	2	1	0	1	2	3	2	3	1	2	3	2	3	4	3	4
20	3	5	5	4	4	2	3	4	4	5	4	5	4	3	4	4	3	2	1	0	1	2	3	4	2	3	2	3	4	3	2	5
21	4	5	4	3	4	3	2	3	5	6	5	5	5	4	4	4	3	3	2	1	0	1	2	3	3	2	1	2	3	2	1	6
22	5	4	5	4	3	4	3	4	6	7	5	6	5	4	5	5	4	4	3	2	1	0	1	2	2	3	2	3	2	3	2	7
23	4	3	4	5	2	3	4	3	5	6	4	5	4	3	5	5	4	3	2	3	2	1	0	1	1	2	3	2	1	2	3	6
24	5	4	3	4	3	4	3	2	5	6	4	5	4	3	4	4	3	2	3	4	3	2	1	0	2	1	2	3	2	3	4	6
25	3	4	5	4	3	2	3	4	4	5	4	5	4	3	4	4	3	2	1	2	3	2	1	2	0	3	4	3	2	3	4	5
26	4	3	2	3	2	3	2	1	4	4	3	3	3	2	3	3	2	1	2	3	2	3	2	1	3	0	1	4	3	2	3	4
27	5	4	3	4	3	4	3	2	5	6	4	5	4	3	4	4	3	2	3	2	1	2	3	2	4	1	0	3	4	3	2	6
28	2	3	4	3	2	1	2	3	3	4	4	5	4	3	4	4	3	3	2	3	2	3	2	3	3	4	3	0	1	2	1	5
29	3	2	3	4	1	2	3	2	4	5	3	4	3	2	5	5	4	4	3	4	3	2	1	2	2	3	4	1	0	1	2	5
30	4	3	2	3	2	3	2	1	5	4	4	5	4	3	4	4	3	3	4	3	2	3	2	3	3	2	3	2	1	0	1	5
31	3	4	3	2	3	2	1	2	4	5	5	4	5	4	3	3	2	3	3	2	1	2	3	4	4	3	2	1	2	1	0	5

Table 6. The number of pair vertices of chalcopyrite structure that are at distance k of each other

Diameter (G) = 7

The Hosoya polynomial is

$H(G,x) = \sum_{k=0}^{7} d(G,k)x^k = 31 + 52x + 118x^2 + 149x^3 + 102x^4 + 37x^5 + 6x^6 + x^7$

To find the Wiener index, we have

$W(G) = H'(G, x)|_{x=1}$

$H'(G, x) = 52 + 236x + 447x^2 + 408x^3 + 185x^4 + 36x^5 + 7x^6$

$W(G) = H'(G, x)|_{x=1} = 52 + 236 + 447 + 408 + 185 + 36 + 7 = 1371$

To calculate the hyper-Wiener index is

$WW(G) = \frac{1}{2}(xH(G,x))''|_{x=1}$

Now, $xH(G,x) = 31x + 52x^2 + 118x^3 + 149x^4 + 102x^5 + 37x^6 + 6x^7 + x^8$.

Then $(xH(G,x))' = 31 + 104x + 354x^2 + 596x^3 + 510x^4 + 222x^5 + 42x^6 + 8x^7$

$(xH(G, x))'' = 104 + 708x + 1788x^2 + 2040x^3 + 1110x^4 + 252x^5 + 56x^6$

$WW(G) = \frac{1}{2}(104 + 708 + 1788 + 2040 + 1110 + 252 + 56)$

$= 3058$.

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