ENERGY AND LAPLACIAN SPECTRUM OF C₄C₈(S) NANOTORI AND NANOTUBE

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The spectrum of a finite graph is by definition the spectrum of the adjacency matrix, that is, its set of eigenvalues together with their multiplicities. The sum of the absolutes of these eigenvalues is the energy of graph. The Laplace spectrum of a finite undirected graph without loops is the spectrum of the Laplace matrix. There are some topological indices related the Laplacian spectrum. In this paper, using a mathematical model for $C_4C_8(S)$ that introduced in Ref.[26], we write a MATHEMATICA program to compute the energy and Laplacian spectrum of molecular graph of arbitrary $C_4C_8(S)$ nanotori and nanotube.

1. Introduction

A topological index is a real number related to a structural graph of a molecule. It does not depend on the labeling or pictorial representation of a graph. In recent years there has been considerable interest in the general problem of determining topological indices of nanotubes, nanotori and fullerenes. It has been established, for example, that the Wiener and hyper-Wiener indices of polyhex nanotubes and tori are computable from the molecular graph of these structures. Accordingly, some of the interest has been focused on computing topological indices of these nanostructures[1,2].

Let G be a undirected graph without directed and multiple edges, and without loops, the vertex and edge-sets of which are presented by $V(G)$ and $E(G)$, respectively. The adjacency matrix of G is the *0-1* matrix $A=A(G)=[a_{ij}]$ indexed by the vertex set $V(G)$ of G, where $a_{ij}=1$ when ij is an edge and $i \neq j$, and *0* otherwise. This matrix characterizes a graph up to isomorphism. It allows the reconstruction of a graph and is a symmetric matrix. The Laplacian matrix of G is the matrix $L=L(G)=[l_{ij}]$ indexed by the vertex set of G, with zero row sums, where $L_{ij}=-a_{ij}$ for $i \neq j$. If $D=D(G)=[d_{ij}]$ is the diagonal matrix, indexed by the vertex set of G such that d_{ii} is the degree of i, then $L=D-A$.

The Laplacian matrix is sometimes also called the Kirchhoff matrix[3] of a graph because of its role in the matrix-tree theorem[4] implicit[5] in the work of Kirchhoff[6]. And sometimes $L(G)$ is called the combinatorial Laplacian, to distinguish it from the normalized Laplacian earlier noted in connection with random walks.

The Laplacian matrix is a real symmetric matrix, so that diagonalization of the Laplacian matrix of a graph (molecule) G with N vertices (atoms) gives N real eigenvalues $\mu_i(G)$, $i=1,2,...,N$. The smallest eigenvalue of the Laplacian spectrum is always *0*, as a consequence of the special structure of the Laplacian matrix. The sum of these eigenvalues is the trace of L, which is twice the number of edges of G. The uses of the Laplacian matrix, its characteristic polynomial, its eigenspectrum, and related invariants have been explored in chemistry for at least the last decade[7-20]. There are many problems in physics and chemistry where the Laplacian matrices of graphs and their spectra play the central role. Some of the applications are mentioned in [21].

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A graph G is called regular of degree k, when every vertex has precisely k neighbors. If G is regular of degree k, then for every eigenvalue θ we have $|\theta| \leq k$ and $L(G)=kI-A(G)$. It follows that if G has ordinary eigenvalues $k= \theta_1 \geq \theta_2 \geq \ldots \geq \theta_N$ and Laplace eigenvalues $0=\mu_1 \leq \mu_2 \leq \ldots \leq \mu_N$, then $\theta_i=k- \mu_i$ for $i=1,2,\ldots, N$. Moreover k is the largest eigenvalue of G, and its multiplicity equals the number of connected components of G.

The Quasi-Wiener index, W^*, defined as $W^*=N \sum_{i=2}^{N} 1/\lambda_i$, where λ_i, $i=2,\ldots,N$ denotes the positive eigenvalues of the Laplacian matrix[3,10].

The eigenvalues of the Laplacian matrix are used in calculating the number of spanning trees, $t(G)$, in graph. We know that if G be an undirected graph with Laplacian matrix $L(G)$ and eigenvalues $0=\mu_1 \leq \mu_2 \leq \ldots \leq \mu_N$, then the number of spanning trees of G, equals [3] $t(G)=\dfrac{\prod_{i=2}^{N} \mu_i}{N}$. Moreover Mohar defined two topological indices, TI_1 and TI_2 on the ground of Laplacian spectrum $TI_1 =2N \, log(Q/N) \sum_{i=2}^{N} 1/\mu_i$ and $TI_2=4/(N \mu_2)$, where Q is the number of edges.

The eigenvalues of adjacency matrix $A(G)$ are called eigenvalues of graph G [4]. Following Ivan Gutman [22], the energy, $E(G)$, of a molecular graph G is defined to be the sum of the absolutes of the eigenvalues of G. We encourage the reader to consult papers [22-24] and references therein for background material as well as basic computational techniques.

A C_4C_8 net is a trivalent decoration made by alternating squares C_4 and octagons C_8. It can cover either a cylinder or a torus. Such a covering can be derived from a square net by the leapfrog operation[25]. Optimized C_4C_8 net covering a nanotube is illustrated in Figure 1. A nanotorus is a nanotube whose ends are connected.
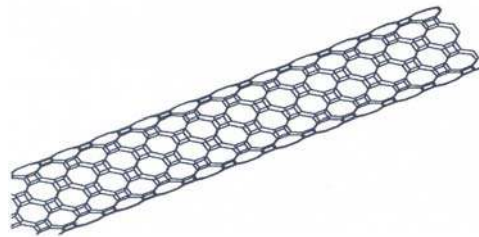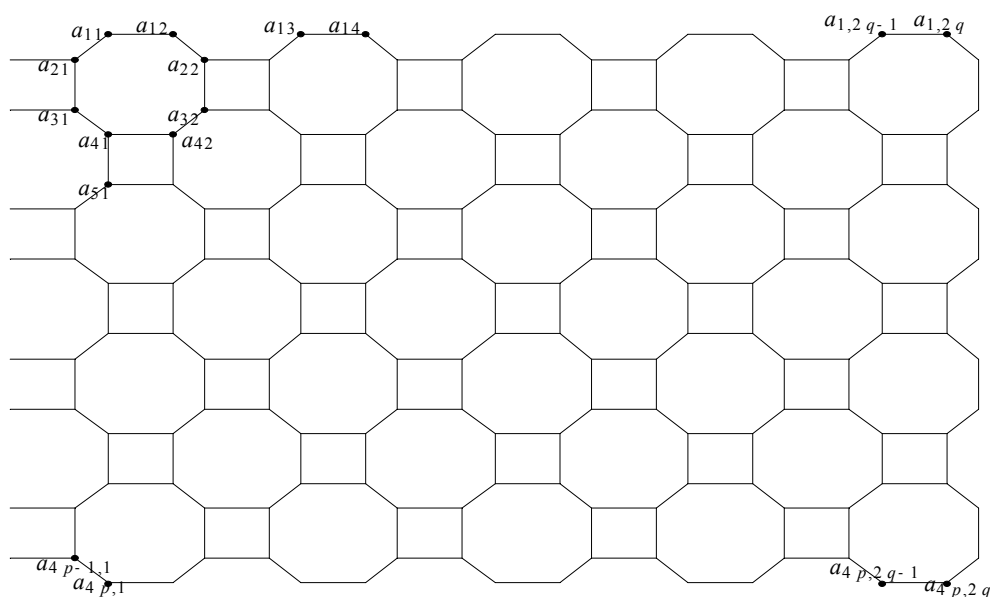

Fig.1. TUC$_4$C$_8$(S).

Fig.2. Two-dimensional lattice of nanotube $G_2=TUC_4C_8(S)$ [4,5].

2. Results and discussions

Description of molecular graphs of nanotori and nanotubes

A carbon nanotorus may be described as a long rolled-up graphite sheet bent around to the form of torus. Let $G_1=TRC_4C_8(S)[p,q]$ and $G_2=TUC_4C_8(S)[p,q]$ be the molecular graphs of $C_4C_8(S)$ nanotorus and nanotube, in which p and q are the number of octagons in vertical and horizontal directions, respectively, Figure 2. Note that the graph G_1 has exactly *8pq* vertices and is a *3*-regular graph and so the Laplacian matrix of this graph is $L(G_1)=3I-A(G_1)$ where I is the $8pq \times 8pq$ identity matrix. Arezoomand and Taeri[26] proved that the set $\ell = \{(\alpha,\beta,\gamma,\delta) \in Z^4 \mid \beta+\gamma+\delta \in \{0,1\}, \alpha+\gamma+\delta \in \{0,1\}\}$ is a mathematical model for vertices of $C_4C_8(S)$ lattice and the mapping $f : \ell \times \ell \to N$, $f(u,v) = \sum_{i=1}^{4} |u_i - v_i|$ is a distance function on the set of lattice vertices and give us the minimum distance between two vertices u and v. We assume that a_{ij} denotes *(i,j)*-entry of two-dimensional lattice of G_2 as shown in Figure 2. We put the origin point O at the a_{41} and consider the vectors e_0, e_1, e_2 and e_3.

Consider the points $a=a_{11}$, $b=a_{21}$, $c=a_{31}$, $d=a_{41}=O$, $e=a_{12}$, $f=a_{22}$, $g=a_{32}$ and $h=a_{42}$. It is easy to see that every point of G_2 can be constructed by a translation of these points in two directions $v=2e_0-e_2+e_3$ and $w=2e_1-e_2-e_3$. This is the content of lemma below.

Lemma 1. Assume that a_{ij}, $1 \le i \le 4p$ and $1 \le j \le 2q$, denotes the *(i,j)*-entry of the two-dimensional lattice of G_2, as shown in the Fig.2, in our model we have

$$a_{ij} = \begin{cases} a_{ij}^1 & i \equiv 1 \pmod 4, j \ odd \ or \ i \equiv 3 \pmod 4, j \ even \\ a_{ij}^2 & i \equiv 1 \pmod 4, j \ even \ or \ i \equiv 3 \pmod 4, j \ odd \\ a_{ij}^3 & i \equiv 2 \pmod 4, j \ odd \ or \ i \equiv 0 \pmod 4, j \ even \\ a_{ij}^4 & i \equiv 2 \pmod 4, j \ even \ or \ i \equiv 0 \pmod 4, j \ odd \end{cases} \quad (1)$$

where

$a_{ij}^1 = (j-1) e_0+(i-3)/2 \ e_1+(7-i-2j)/4 \ e_2+(3-i+2j)/4 \ e_3,$

$a_{ij}^2 = (j-1) e_0+(i-3)/2 \ e_1+(9-i-2j)/4 \ e_2+(1-i+2j)/4 \ e_3,$

$a_{ij}^3 = (j-1) e_0+(i-4)/2 \ e_1+(8-i-2j)/4 \ e_2+(-i+2j)/4 \ e_3$

and

$a_{ij}^4 = (j-1) e_0+(i-4)/2 \ e_1+(6-i-2j)/4 \ e_2+(2-i+2j)/4 \ e_3.$

Proof. It is easy to see that the lattice points of G_2 lie in $T_1 \bigcup T_2 \bigcup \ldots \bigcup T_8$, where

$T_1 = \{a+ (i-1)/4 \ w+ (j-1)/2 \ v \mid i \equiv 1 \ (mod \ 4), j \ odd\}$
$T_2 = \{e+ (i-1)/4 \ w+ (j/2-1) \ v \mid i \equiv 1 \ (mod \ 4), j \ even\}$
$T_3 = \{b+ (i-2)/4 \ w+ (j-1)/2 \ v \mid i \equiv 2 \ (mod \ 4), j \ odd\}$
$T_4 = \{f+ (i-2)/4 \ w+ (j/2-1) \ v \mid i \equiv 2 \ (mod \ 4), j \ even\}$
$T_5 = \{c+ (i-3)/4 \ w+ (j-1)/2 \ v \mid i \equiv 3 \ (mod \ 4), j \ odd\}$
$T_6 = \{g+ (i-3)/4 \ w+ (j/2-1) \ v \mid i \equiv 3 \ (mod \ 4), j \ even\}$
$T_7 = \{d+ (i/4-1) \ w+ (j-1)/2 \ v \mid i \equiv 0 \ (mod \ 4), j \ odd\}$
$T_8 = \{h+ (i/4-1) \ w+ (j/2-1) \ v \mid i \equiv 0 \ (mod \ 4), j \ even\}$

By considering the coordinates of the points a, b, c, d, e, f, g, h and the vectors v, w we can see that the relation (1) holds.

Note that in the $C_4C_8(S)$ net the nearest neighbors of vertex $v=(v_1,v_2,v_3,v_4)$ are

$v^1 = (v_1 + \varepsilon_1(v), v_2, v_3, v_4)$
$v^2 = (v_1, v_2 + \varepsilon_2(v), v_3, v_4)$ $\qquad (1)$
$v^3 = (v_1, v_2, v_3 + \varepsilon_{31}(v), v_4 + \varepsilon_{32}(v))$

where

$$\varepsilon_1(v) = (-1)^{v_1+v_3-v_4}$$
$$\varepsilon_2(v) = (-1)^{v_2+v_3+v_4}$$

$$\varepsilon_{31}(v) = \begin{cases} \varepsilon_2(v) & if \quad v_2 + v_3 + v_4 = v_1 + v_3 - v_4 \\ 0 & otherwise \end{cases}$$

$$\varepsilon_{32}(v) = \begin{cases} \varepsilon_2(v) & if \quad v_2 + v_3 + v_4 \neq v_1 + v_3 - v_4 \\ 0 & otherwise \end{cases}$$

By above notations, it is obvious that if we fix p and q, then $V(G_1)=V(G_2)$ and $E(G_1)=E(G_2)$ $\bigcup \{a_{1j}a_{4p,j} | 1 \leq j \leq 2q\}$.

By the geometry of nanotori we have

$$a_{i1}^1 = a_{i,2q} \text{ (and so } a_{i,2q}^1 = a_{i1} \text{) when i=2 or 3 (mod 4)}$$

$$a_{1j}^2 = a_{4p,j} \text{ (and so } a_{1j}^2 = a_{4p,j} \text{) for all j.}$$

Note that we can compute the other neighbors of these vertices and all of neighbors of other vertices by relations (1).

A MATHEMATICA program for computing the adjacency and Laplacian matrices of G_1 and G_2.
Now we are ready to write a MATHEMATICA program for computing the adjacency and Laplacian matrices of $C_4C_8(S)$ nanotori and nanotubes. Using these two important matrices we can compute some topological indices. In the output of our program $V=V(G_1)=V(G_2)$, *A1* and *A2* are the adjacency matrices of G_1 and G_2, respectively. Also *L1* and *L2* are the Laplacian matrices of G_1 and G_2, respectively and *Eig1*, *Eig2* are the set of their eigenvalues. Finally *D2* is the degree matrix of G_2.

```
p=4; q=5;(* for example*)
a = {0, -1, 1, 1}; b = {0, -1, 1, 0}; c = {0, 0, 1, 0}; d = {0, 0, 0, 0}; e = {1, -1, 1, 1}; f = {1, -1, 0,
1}; g = {1, 0, 0, 1}; h = {1, 0, 0, 0};v={2, 0, -1, 1}; w = {0, 2, -1, -1};
 V = {};
 For[i=1, i≤ 4p,
   For[j=1, j≤ 2q,
     If[Mod[i,4]==1 && OddQ[j], AppendTo[V, a+ (i-1)/4w+ (j-1)/2v]];
     If[Mod[i,4]==1 && EvenQ[j], AppendTo[V, e+ (i-1)/4w+ (j/2-1)v]];
     If[Mod[i,4]==2 && OddQ[j], AppendTo[V, b+ (i-2)/4w+ (j-1)/2v]];
     If[Mod[i,4]==2 && EvenQ[j], AppendTo[V, f+ (i-2)/4w+ (j/2-1)v]];
     If[Mod[i,4]==3 && OddQ[j], AppendTo[V, c+ (i-3)/4w+ (j-1)/2v]];
     If[Mod[i,4]==3 && EvenQ[j], AppendTo[V, g+ (i-3)/4w+ (j/2-1)v]];
     If[Mod[i,4]==0 && OddQ[j], AppendTo[V, d+ (i/4-1)w+ (j-1)/2v]];
     If[Mod[i,4]==0 && EvenQ[j], AppendTo[V, h+ (i/4-1)w+ (j/2-1)v]];
     j++];
   i++];
A1 = Table[x[i, j], {i, 1, 8p*q}, {j, 1, 8p*q}];
 ff[u_, v_] :=Sum[Abs[u[[i]] - v[[i]]], {i, 1, 4}];
 For[i = 1, i ≤  8p*q,
   For[j = 1, j ≤  8p*q,
     If[ff[V[[i]], V[[j]]] = = 1, x[i, j] = 1, x[i, j] = 0];
     j++];
   i++];
For[i = 1, i ≤  2q,
   x[i, (8p-2)q + i] = 1;
   x[(8p-2)q+ i, i] = 1;
 i++];
For[i = 0, i ≤p-1 ,
    x[(8i+2)q+1,(8i+4)q] = 1;
   x[(8i+4)q, (8i+2)q+1] = 1;
x[(8i+4)q+1,(8i+6)q]=1;
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```
x[(8i+6)q, (8i+4)q+1]=1;
 i++];
A2 = Table[z[i, j], {i, 1, 8p*q}, {j, 1, 8p*q}];
For[i= 1, i≤ 8p*q,
   For[j = 1, j ≤ 8p*q,
     If[ff[V[[i]], V[[j]]] = = 1, z[i, j] = 1, z[i, j] = 0];
   j++];
  i++];
For[i = 0, i ≤p-1 ,
    z[(8i+2)*q+1,(8i+4)*q] = 1;
    z[(8i+4)*q, (8i+2)*q+1] = 1;
    z[(8i+4)*q+1,(8i+6)*q]=1;
    z[(8i+6)*q, (8i+4)*q+1]=1;
 i++];
D2 = Table[dd[i, j], {i, 1, 8p*q}, {j, 1, 8p*q}];
B=A2.A2;
 For[i = 1, i≤ 8p*q,
    For[j = 1, j≤ 8p*q,
        If[i= =j, dd[i,j]=B[[i]][[j]], dd[i,j]=0]
      j++]
   i++]
L1=3*IdentityMatrix[8p*q] - A1;
L2=D2-A2;
Eig1=Eigenvalues[L1]//N
Eig2=Eigenvalues[L2]//N
```

Topological indices and energy of nanotori and nanotube
It is easy to see that $|E(G_1)| = 12pq$ and so $|E(G_2)|=12pq-2q$. Note that MATHEMATICA arranges the Laplacian eigenvalues decreasing. So if we append these below lines to the program, then we have numerical values of the topological indices W^*, TI_1, TI_2, the number of spanning trees $t(G)$, μ_2 (as defined in the section 1) and energy of nanotori and nanotube :

```
(*for nanotori*)
Eig1[[8p*q-1]]
QuasiWiener1 = 8p*q*Sum[1/Eig1[[i]], {i, 1, 8p*q - 1}]
tG1=Product[Eig1[[i]], {i, 1, 8p*q - 1}]/(8p*q)
TI1G1 =16p*q*Log[4/3]*Sum[1/Eig1[[i]], {i, 1, 8p*q - 1}]
TI2G1 =4/(8p*q*Eig1[[8p*q - 1]])
E1=Eigenvalues[A1];
EnG1=Sum[Abs[E1[[i]]],{i,1,8p*q}]//N
(*for nanotube*)
Eig2[[8p*q-1]]
QuasiWiener2=8p*q*Sum[1/Eig2[[i]], {i, 1, 8p*q - 1}]
tG2=Product[Eig2[[i]], {i, 1, 8p*q - 1}]/(8p*q)
TI1G2=16p*q*Log[4/3-1/(4p)]*Sum[1/Eig2[[i]], {i, 1, 8p*q - 1}]
```

Table1. Numerical data for nanotorus $G_1=TRC_4C_8(S)[p.q]$.

(p,q)	μ_2	W^*	t(G)	TI_1	TI_2	Energy
(2,2)	0.585786	550.476	6.04231×10^{10}	316.724	0.213388	47.5717
(2,3)	0.267949	1431.07	1.58582×10^{16}	823.386	0.311004	70.4683
(2,4)	0.152241	2887.15	3.68402×10^{21}	1661.16	0.410533	94.9648
(2,5)	0.097887	5046.16	8.02232×10^{26}	2903.38	0.510793	118.667
(2,6)	0.0681483	8036.07	1.67705×10^{32}	4623.67	0.611411	141.951
(2,7)	0.0501442	11984.9	3.40847×10^{37}	6895.67	0.712232	166.048
(2,8)	0.0384294	17020.6	6.78606×10^{42}	9793.03	0.813179	189.752
(3,2)	0.267949	1431.07	1.58582×10^{16}	823.386	0.311004	70.4683
(3,3)	0.267949	3472.83	2.78463×10^{24}	1998.14	0.207336	105.091
(3,4)	0.152241	6681.15	4.17439×10^{32}	3844.09	0.273689	141.202
(3,5)	0.097887	11240.5	5.84076×10^{40}	6467.38	0.340529	176.487
(3,6)	0.0681483	17340.5	7.84154×10^{48}	9977.1	0.407608	211.343
(5,2)	0.097887	5046.16	8.02232×10^{26}	2903.38	0.510793	118.667
(5,3)	0.097887	11240.5	5.84076×10^{40}	6467.38	0.340529	176.487
(5,4)	0.097887	20573.1	3.12427×10^{54}	11837	0.255397	235.557
(5,5)	0.097887	33369.5	1.49478×10^{68}	19199.6	0.204317	294.493

Table2. Numerical data for nanotube $G_2=TUC_4C_8(S)[p.q]$.

(p,q)	μ_2	W^*	t(G)	TI_1	TI_2	Energy
(2,2)	0.152241	768.834	6.25766×10^{8}	290.991	0.821067	45.5573
(2,3)	0.152241	1873.15	1.8522×10^{13}	708.975	0.547378	68.0914
(2,4)	0.152241	3656.07	4.61365×10^{17}	1383.76	0.410533	90.3743
(2,5)	0.097887	6242.33	1.06635×10^{22}	2362.62	0.510793	113.593
(2,6)	0.0681483	9757.05	2.36124×10^{26}	3692.89	0.611411	136.419
(2,7)	0.0501442	14326.9	5.08126×10^{30}	5422.5	0.712232	159.025
(2,8)	0.0384294	20079.4	1.07106×10^{35}	7599.75	0.813179	181.503
(3,2)	0.0681483	2079.59	1.09013×10^{14}	928.094	1.22282	69.5174
(3,3)	0.0681483	4639.42	2.07274×10^{21}	2070.51	0.815215	103.625
(3,4)	0.0681483	8587.9	3.05379×10^{23}	3832.67	0.611411	138.068
(3,5)	0.0681483	14131.3	4.05566×10^{35}	6306.62	0.489129	172.728
(3,6)	0.0681483	21459.5	5.10528×10^{42}	9577.08	0.407608	206.981
(5,2)	0.0246233	7833.78	3.30835×10^{24}	3908.44	2.0306	116.802
(5,3)	0.0246233	15752.5	2.59415×10^{37}	7859.26	1.35373	174.045
(5,4)	0.0246233	27238.3	1.32995×10^{50}	13589.8	1.0153	231.991
(5,5)	0.0246233	42748.7	5.74189×10^{62}	21328.3	0.812238	290.519
(5,6)	0.0246233	62673.6	2.27372×10^{75}	31269.2	0.676865	348.268

TI2G2=4/(8p*q*Eig2[[8p*q - 1]])
E2=Eigenvalues[A2];
EnG2=Sum[Abs[E2[[i]]],{i,1,8p*q}]//N

We give a numerical data for these indices, number of spanning trees and energies of the graphs G_1 and G_2 in Tables 1, 2. After running the above programs, we can guess some conjectures as follows:

Conjecture1. After running our program in many cases for p and q, we guess that the characteristic polynomial of Laplacian matrix of G_1 is of the form $f(x) = (x - \mu_1)^{\alpha_1}(x - \mu_2)^{\alpha_2}...(x - \mu_k)^{\alpha_k}$ where $0=\mu_1<\mu_2<...<\mu_k=6$ are distinct eigenvalues of Laplacian matrix with multiplicity α_i, $1\leq i\leq k$, respectively, $\sum_{i=1}^{k}\alpha_i =|V(G_1)|$, $\alpha_1=\alpha_k=1$ and for $1\leq j \leq [k/2]$, $\alpha_{k-j+1}=\alpha_j$.

Conjecture2. If we fix p and q, then we have $E(G_1)>E(G_2)$, where $E(G)$ is the energy of graph G.

3. Conclusions

In this work, we give a MATHEMATICA program for calculating two important matrices adjacency and Laplacian of arbitrary $C_4C_8(S)$ nanotorus and nanotubes. Many structural properties of these nanostructures are depending to these matrices. The molecular graph of these structures is given as an algebraic definition. Similarly one can write simple MATHEMATICA program and compute many topological indices related with these matrices, such as Randic index, Zagreb group indices, etc. Moreover according Huckel theory we can equate the eigenvectors of the adjacency matrix for atomic orbitals in the construction of molecular orbitals. Also we can use the eigenvectors for analyze some physico-chemical properties and interesting intra-and inter-molecular ordering (for more details see Refs. [27, 28]) .

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