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Visualization and Simulation of Carbon Structures with Higher Genus

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***Abstract*—The Computational Science Initiative (CSI) department at Brookhaven National Laboratory involves varied and interdisciplinary work through out all sciences. In particular, we worked within the realm of computational chemistry through the means of studying carbon nanotori structures via their visualization and simulation. Compounds like graphene and other carbon allotropes,such as the nanotorus, have been in the eye of scientists for several years due to their unique polyhex structures which provide unique topologies and therefore possibly unique material properties. C++ code to generate Cartesian coordinates for an arbitrary torus was utilized to allow the use of molecular editing and modeling programs, such as Avogadro or Visual Molecular Dynamics (VMD) to design multiple genus nanocarbon toroidal structures. Several files were generated that contained multiple genus to them, namely a double torus, triple torus, and quadruple torus, all based off of a single genus carbon nanotorus from previous said code. Bond angle information was then utilized through .report files generated from structures files (.xyz or .cml) to allow for vertices and thereby neighboring atoms to the vertices to be identified. With these identified atoms for the above multiple genus structures, as well as for the C240 buckyball fullerene and carbon nanotorus, we wrote C++ code to generate an adjacency matrix for each respective one. These matrices were then subsequently used to generate eigenvalues and eigenvectors through a Mathmatica function for each structure. Using these values we can study the energies of these systems and thereby its functionalities and properties.**

***Index Terms*—carbon, carbon nanotube, visualization**

I. Introduction

A. An Introduction to Fullerenes

Nanocarbon structures like fullerenes have been a hot area of study for most facets of science ever since their advent in the 1980's. [1] In a sense, these structures prompt the question of just how important a structures topology is to its physical properties. These properties being varied and diverse, such as conductivity, transmission of light, and reactions to magnetic fields. [2] To start, we should define formally what a fullerene is and what makes it distinct from other allotropes of carbon. Carbon 60 (C_{60}) buckminsterfullene, also known as the buckyball, obtained its name from the geodesic dome structures made by architect Buckminster Fuller. The fullerene, (C_N), can be defined as a carbon polyhedron with 12 pentagonal and N/2 10 hexagonal faces, with plausible values of N ranging from 20 to $\geq$ 70 Carbon atoms. [1] Even though typically fullerenes are meant to reference spherical, ball-like structures under the above rule, some also apply the definition to other allotropic topologies of carbon, like the carbon nanotube or carbon nanotorus. All of these nanocarbon structures can be described through the Euler's polyhedral formula for N-vertex trivalent spherical polyhedrons:

$$V + F = E + 2. \tag{1}$$

Where V = N with f being the number of vertices, E = 3N / 2, where e is the number of edges. Therefore F = (N / 2) + 2, which allows for the Poincaré formula to be used for genus 1 structures, like fullerenes. [1]

$$\sum_r (6-r)F_r = 3F_3 + 2F_4 + F_5 - F_7 - 2F_8 - ... = 12. \tag{2}$$

Or in a general form

$$\sum_r (6-r)F_r = 12(1-g) \tag{3}$$

where r is the number of vertices on the boundary of the faces, F is the number of faces, and g is the genus of the structure. [1]

There is also the relationship for a nanotube system with open ends:

$$\sum_r (6-r)F_r = 12(1-g) - 6H \tag{4}$$

where H is the number of open ends. [3]

B. Other Carbon Nanostructures

Aside from the fullerene, there are other carbon nanostructures of great interest to scientists although due to similar topological basis. One such structure is the carbon nanotube. This structure, like the name implies, is a tube composed of a carbon sheet. More specifically though, this can be conceptualized as involving a parallelogram or rectangle excised of a carbon nanosheet a graphene sheet. This graphene sheet is then rolled up via connecting either opposite edge to one another

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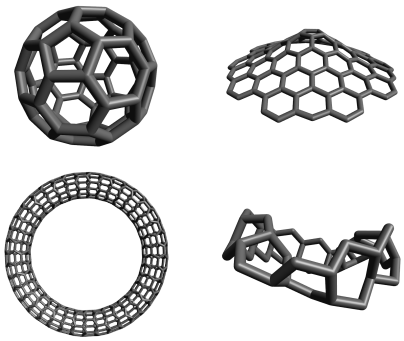

Fig. 1: Stick models created in Avogadro (v1.2.0) on various nanocarbon allotropes. Top left structure is carbon 60 (C_{60}) fullerene. Bottom left structure is (C_{480}) zigzag (6,0) nanotorus. Top right structure is (C_{115}) nanocone with one pentagon at its tip. [4] Bottom right is a carbon 48 (C_{48}) polyacene mobius strip structure. [5]

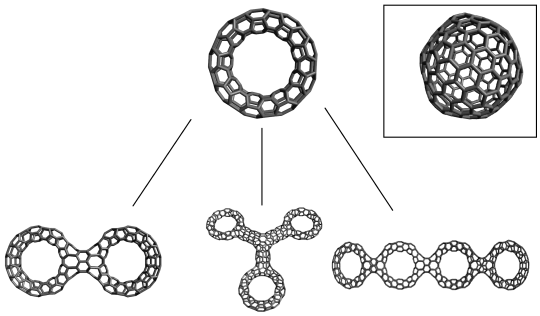

Fig. 2: (C_{144}) zigzag (4,0) nanotorus (top) used to make (C_{300}) double nanotorus (left), (C_{570}) triple nanotorus (middle), and (C_{644}) quadruple nanotorus (right). Top right structure was a preset model in avogadro, (C_{240}) fullerene. All structures were modeled in Avogadro (v 1.2.0).

allowing for a carbon nanotube shape. Now from the nanotube shape one can then see how by simply connecting the ends of a nanotube they can yield a toroidal shape; a carbon nanotorus.

As per the Poincaré formula, one can see that the genus of a surface, the number of holes a surface has, can differ between polyhedral shapes and therefore carbon nanostructures. [1] If one considers the surface of a fullerene or sphere, or an infinite plane, these surfaces all are of genus zero. Where as other structures, such as the open carbon nanotube previously described, would have a genus of one as well as the simple carbon nanotorus. There also exists several other nanocarbon allotropes with varied and interesting topologies, such as nancones or a polyacene mobius strip as seen in figure 1.

C. Multiple genus carbon nanotorus

Carbon nanotori are thought to have just as much functionality for applications as carbon nanotubes, if not more, due to their topology. Examples can be seen through its elasticity allowing for development of flexible nanodevices as well as its putative role in electromagnetic oscillators. Being toroidal also allows it the utility to trap particles within its structure. [6] As one can see from figure 1, there exists carbon nanostructures with more than one genus. If the genus of a structure can be defined as the amount of handles one can add to a surface then one would reason that by adding handles to a surface, one can increase the genus of the structure. More specifically if one added a torus to a surface, such as another torus, this can allow for structures with respectively increasing genus. This was one of the roles within our project, to design multiple genus carbon nanotori structures. Examples can be seen in figure 2. [7]

In order for me to connect these handles and create the extra genus, we needed to use the proper attachments. This was necessary for even though a single torus can be created with all hexagons, it needs imperfections in the form of non hexagonal tiling to allow for any other connections. This can be seen again through the Poincaré formula for any multiple genus toroidal structure. As an example, to make a double torus structure with all hexagons would yield the following result, which is not valid.

$$\sum_r (6-r)F_r = 12(1-g) \tag{5}$$

$$0 \neq 12(1-g)$$

Where as for a single torus:

$$\sum_r (6-r)F_r = 12(1-1) \tag{6}$$

One can see other valid topologies for simple nanotori through introduction of imperfections within the structure itself, such as a certain ratio of heptagons to pentagons or simply a torus made fully of pentagons and hexagons. [6]This is a result of these non-hexagonal tiling having a different surface area than the traditional hexagon a pentagon with a smaller area allows for the introduction of positive curvature for a structure which then must be balanced with larger surface area tiling, such as a heptagon, which introduces negative curvature. However, non-hexagonal tiling can result in kinks in a structure which can allow for trapped particles, which leaves the designer many considerations when conceptualizing nanostructures. [6] This is why through the use of special carbon nanojunctions as my proper connections it could compensate for the Poincaré formula and construct valid topologies of multiple genus toroidal structures. Examples of these junctions can be seen in figure 3. [7], [8]

However, we could not just add the junctions, for that would ruin the trivalent bonds that are normally found in graphene sheet structures. Therefore, we made holes in the carbon nanotori structures prior to junctioning to allow for the retention of the trivalent bonds, with respect to the size of the junction.

II. Methods

A. Design of Carbon Nanostructures

As stated above, we needed to design carbon nanotoroidal structure of multiple genus. This process was to be an extension of work done by Low and McGuigan on visualizing a

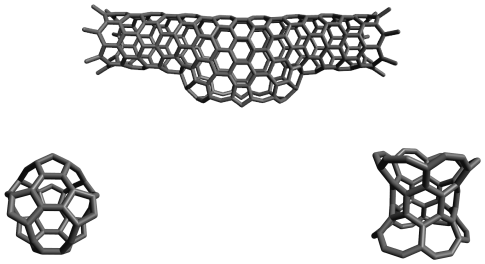

Fig. 3: Junctions made in Avogadro (v1.2.0) for joining carbon structures. Bottom left is a octagon/pentagon (6/6) based y junction, used in the triple torus. Top is a heptagon/pentagon (8/2) based T-Junction (not used). Bottom right is a 12 pentagon wormhole junction, used in the double and quadruple nanotorus. [9]–[11] Note x junction was not shown. [12]

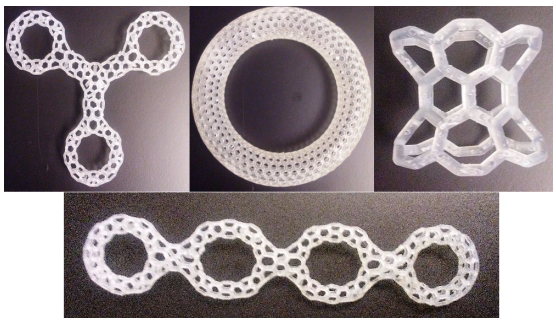

Fig. 4: 3D structures of a triple, single, quadruple nanotorus, (top left, top, bottom) and wormhole junction (top right); printed via .stl files from VMD. [8]

carbon nanotorus of genus 1 through 3D coordinates via C++ code based off of a graphene lattice. [13] These Cartesian coordinates could then be drawn through chemistry software such as VMD (version 1.9.3) or Avogadro (version 1.2.0). [7], [8] These molecular editors allow for hands on visualizing of 3D molecular structures, along with direct manipulation of structures via rotations and transformations. VMD and Avogadro each also had their own user friendly functions such as but not limited to: copy, cut, paste, and drag and drop options for molecules and whole structures alike. Having these options, along with the the nanotube and graphene sheet builder from VMD and the fullerene library from Avogadro all facilitated my design process. Currently we do not have C++ code for generating multiple genus carbon toroidal structures since we took a different approach to generate our current multiple genus structures. I found it simpler to use the editing tools provided by VMD and Avogadro to directly manipulate coordinates for forming toroidal structures. We were able to design multiple junctions as well as multiple genus nanotori structures, as evidenced by figure 2 and 3. In addition, 3D prints are also viable through .stl files generated by VMD as seen in Figure 4.

B. Adjacency Matrices, Eigenvalues and Eigenvectors

From our structures made we quantified the relations between the carbon atoms through the use of an adjacency matrix. Given a set of elements, which can be taken as the vertices of a bond, one can find then adjacent neighboring atoms to those vertices. This then allows for the connectivity of structure to be described through matrix form. To start, given my structures were all made through Avogadro, we needed a way to export the bond angle information to which Avogadro did not support. By taking .cml files from Avogadro and pushing them through OpenBabel (version 2.3.1), software for chemical file analysis and conversion, we were able to generate this bond angle information via a .report file. [14] For a trivalent carbon structure, this bond angle information yielded redundant, but usable data on neighboring atoms to each vertex. To detail my process, The adjacency matrix program needed the numerical data from a .report file under the "BOND ANGLE" section of an OpenBabel generated .report file, which was subsequently generated by converting from .cml or .xyz formats. This section's data can be manually copy and pasted into a .txt file in the C++ project folder of the program, with the file labeled bondList.txt. An Adjacency matrix is then generated for the neighboring carbon atoms of a structure with three bonds to each respective carbon and saved in a user defined .txt file upon running the console application.

Parsing these data with C++ code allowed for the generation of adjacency matrices on the following structures, a (C_{240}) Buckyball fullerene (genus zero), a (C_{144}) nanotorus (genus one), a (C_{300}) double nanotorus (genus two), a (C_{570}) triple nanotorus (genus three), and lastly a (C_{644}) quadruple nanotorus (genus four). Each respective adjacency matrix was listed as a set of sets. That is for every carbon atom there is a set to describe each adjacent carbon atom to each vertex in which there should be three since our nanotorus structures are again based on graphene sheets, which have trivalent bonds. With the Mathmatica eigensystem function we were then able to generate the eigenvalues and eigenvectors based upon my adjacency matrices.

III. Data and Results

A summary of some displayed polyhedron attributes is displayed in Table 1. The multiple genus toroidal structures are available in .xyz or .cml form. The (C_{240}) fullerene was a preset structure in Avogadro available for me to use, as well as other fullerenes. To generate ones own .report files off of the .xyz or .cml file formats for viewing one can use OpenBabel software. Currently we have not yet determined the free energy for all of our structures. we are still working on a way to utilize the below formula for the free energy with my eigenvalue and eigenvector data. [16]

$$F(\phi,T) = -\sum {}_{LJ} k_B T \ln(1+\exp[\frac{E_F - E^{(L,J)}_{(\phi,T)}}{k_B T}]) \quad (7)$$

Name	Pentagons	Heptagons	Octagons	Nonagons	Genus	χ
C_{60} fullerene	12	0	0	0	0	2
C_{240} fullerene	12	0	0	0	0	2
C_{144} zigzag (4,0) nanotorus	0	0	0	0	1	0
C_{300} double torus	0	12	0	0	2	-2
C_{570} triple torus	6	18	6	0	3	-4
C_{644} quadruple torus	0	36	0	0	4	-6
C_{60} wormhole junction	0	12	0	0	0	-2
C_{24} x junction	0	0	0	4	0	-2
C_{48} y junction	6	0	6	0	0	-1
C_{270} t junction	2	8	0	0	0	-1

TABLE I: A general list of structures made and their attributes; note that the Euler characteristic was determined via $\sum_r \frac{(6-r)F_r}{6} = \chi = 2(1-g)$, where χ is the Euler characteristic, or for an open structure; $\chi = 2(1-g) - H$ where the genus is 0 and H is the amount of open ends. [15]

Where ϕ is the magnetic flux and T is the temperature in Kelvins, E_F is the Fermi energy, and L, J labels the eigenvalues.

As an aside, eigenvalues and vectors are too large to display in this paper which is why they are not shown. The Eigensystem command was used in Mathmatica to generate the eigenvalues from the adjacency matrix.

IV. Conclusion

Future work can be done on code to generate multiple genus structure so that the computer aided design is not needed. If not, then investigating other modeling software to assist in the design could be another avenue; software like Chemcraft show promise in creating and junctioning structures, but were not used. Also other thermodynamic or electromagnetic properties could and can be investigated through these carbon systems.

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