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Activity

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From Desktop Toy to Educational Aid: Neo Magnets as an Alternative to Ball-and-Stick Models in Representing Carbon Fullerenes

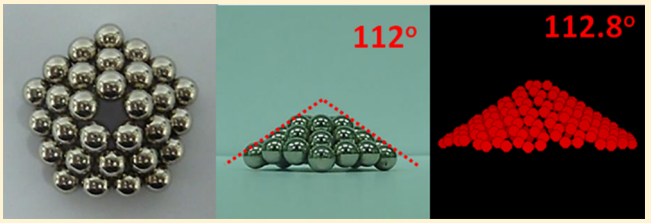
Jacqueline Y. Kao,[†] Min-Han Yang,[‡] and Chi-Young Lee*[,‡]

[†]Science Knowledge Ltd., Taipei 11444, Taiwan, R.O.C.

[‡]Department of Materials Science and Engineering, National Tsing Hua University, Hsinchu 30013, Taiwan, R.O.C.

Supporting Information

ABSTRACT: Neo magnets are neodymium magnet beads that have been marketed as a desktop toy. We proposed using neo magnets as an alternative building block to traditional ball-and-stick models to construct carbon allotropes, such as fullerene and various nanocone structures. Due to the lack of predetermined physical connections, the versatility of carbon bonding can be allowed for when using magnetic beads, as well as providing a more comprehensive appreciation for the angles required for stable bonding within a structure. The students are asked to make neo magnet models of various nanocone structures as well as using software to create the structures, and then compare cone angles obtained with both methods. This activity was trialed on several discussion groups with positive results and feedback of a deeper understanding for carbon nanostructures.



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INTRODUCTION

Carbon is considered the most important element to living things as it is the building block of life and the fourth most abundant element on earth. Its properties allow it to bond to different elements, in different ways to form essential compounds. It gives insight into the wide-ranging properties of carbon materials, as well as carbon's involvement in a plethora of biological reactions. That is the reason for its prominent presence across many disciplines, from chemistry to biology, from material science to biotechnology. Within these disciplines, the bonding chemistry of carbon is often a fundamental topic in the curricula of high school, colleges, and universities around the world.

Carbon uses sp^3, sp^2, and sp hybridization of orbitals to form alkane, alkene, and alkyne bonds in all organic compounds. These are facts commonly found in high school chemistry textbooks[1] as well as those from general chemistry at college level.[2] As for allotropes of carbon, the most prominently featured are graphite and diamond. They are often mentioned in contrast due to their vastly different physical properties, yet having the same elemental composition. Carbon atoms are sp^3-bonded to each other in a tetrahedral formation within diamond, and sp^2-bonded in graphite to form sheets of 6-membered rings. But in reality there are plenty of other allotropes that have more complex structures, which involve different hybridized bonds within a single structure or hybridizations that have varied ratios of s- and p-character and do not conform to the standard sp^3, sp^2, or sp hybridization.[3]

In 1996, a Nobel Prize was awarded for the discovery of C_{60}, buckminsterfullerene. It is a spherical hollow structure composed of 60 carbon atoms, resembling a soccer ball as it is made up of 12 pentagons and 20 hexagons.[4] All carbon bonds in this structure are identical. In order to achieve this geometry, the hybridization of the carbon bonds in C_{60} is somewhere between sp^3 and sp^2. Apart from its interesting properties, its discovery led to the development of a brand new field of chemistry: the study of fullerenes, molecules composed entirely of carbon atoms which take the form of hollow spheres or tubes or various other shapes.[5] Since then, many resources and academics have incorporated C_{60} and other fullerenes into their teaching as examples over the past two decades, particularly under topics regarding chemical or carbon bonding.[6] They are also popular subjects in materials science and engineering, as the bulk properties change with the fullerene structure, for example conductivity and magnetism.[7] Thus, understanding how different structures are formed[8] is pivotal in designing carbon nanostructures with desirable properties for a range of applications.[9,10]

Models are a common method of communicating science. In the case of atoms and molecules, models are representations of things that are too small for direct observation, so that we may interact with them in a manner perceivable by our five senses.[11] Physical models are beneficial to our understanding of science, because one can manipulate and explore their 3D structures. Computerized molecular modeling is extremely useful in constructing with ease molecules of any number or size,[12] and producing 2D or 3D images or even animations. But the information that each individual gains may vary depending on the user's proficiency with computers, which could result in a

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discrepancy in understanding during discussion with other students.[13] Therefore, physical models are still very popular for use in teaching and discussions in science.[11]

Visualizing a three-dimensional molecular structure can be difficult for some, which is why many institutions and studies utilize models to aid in structural visualization. One of the most common types of physical models used is ball-and-stick, where atoms are represented by spheres of various colors with predrilled holes for rods or sticks, which represent bonds. However, with the versatility of carbon bonding, many allotropes, for example fullerene C_{60} and carbon nanocones, cannot be easily built with ball-and-stick models due to the need to accommodate specific bond angle and curvature within the structure. Some have compensated by using basic jewelry-making techniques: putting beads onto a thread to make a buckyball (Figure 1). Threaded beads provide flexible bond angles that can be easily manipulated. However, due to this very flexibility, it is difficult to experience the instability created by any deviation from the stable bond angle. Thus, this method may be entertaining for students, but the understanding and significance of carbon bonding are not clearly communicated.[14] Fortunately, with advancements in computer technology, it is possible to create simulations of such a molecule for the purpose of demonstration. But in this case the hands-on nature of building a model from scratch is lost.

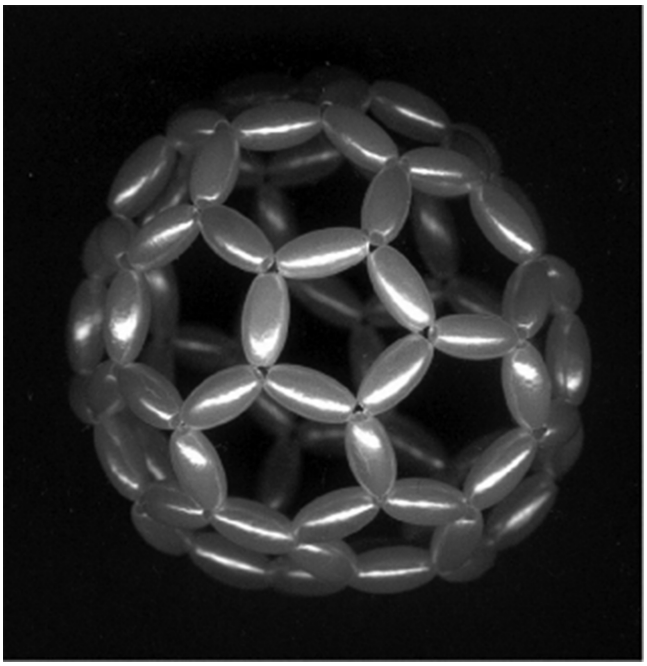

Figure 1. A buckyball made by stringing rice-like beads onto a thread. The beads represent the carbon−carbon bonds.[14]

Researchers have often chosen to use popular toys, such as LEGO blocks, as educational tools in order to illustrate complicated concepts in chemistry because of the public's familiarity with them and their association with fun.[15] For example, catalysis was made easier to understand with LEGO-like building blocks,[16] and the theory of activation energy demonstrated with a slap bracelet.[17] We propose an alternative modeling medium that is also a well-known toy, neo magnets (neodymium magnetic beads), to represent building blocks, held together simply by magnetic force. The hands-on experience is retained, and without predetermined bond positions of the ball-and-stick models, each block can adjust bonding position and angle to form the most stable configuration of a given structure. Neo magnets are relatively inexpensive and readily available to the public as stationery or toys, and there is plenty of information about them on hobbyist Web sites or science blogs.[18] Many videos of tricks performed using these magnets can be found on popular video streaming Web sites, so students should be familiar with them.[19] The idea of using magnetic beads such as these for nanostructure modeling, in particular carbon allotropes, has been previously proposed.[20] The activity described in the present paper includes not only physical modeling but also computer simulations for comparison to provide a more comprehensive understanding of these nanostructures.

■ ACTIVITY DETAIL

As part of any lecture, lab, or workshop on the topic of carbon fullerenes, the instructor can introduce this activity to help students grasp and visualize fullerene structures. "Why do carbon nanostructures adopt their specific shape?" is an example of a focus question that could be asked. An examination of carbon nanostructures such as buckyballs and buckytubes can reveal that any defects in the regular structures result in alterations such as bends and corners, creating variations from the original shape (see more information in Discussion). Nanocones are a great demonstration of "defects" within nanotubes, as their cone angles change when the number of magnets at the apex of each cone deviates from the natural 6. Therefore, in this activity, we will look at how nanostructures maintain stability through specific configurations of their atoms, and the effects on resultant structures when "defects" occur.

There are many ways to build with neo magnets: (i) Form a chain of beads (Figure S3a), at one end make a loop with the desired number of beads as the apex, then wrapping around to create the structure (Figure S3b); or (ii) make individual rings before putting them together. In our experience, method 1 is more suited to nanocone structures with apex rings of 2−6 beads. (See video in Supporting Information I.) For the nanocones with larger apex rings, method 2 was easier; first, make the apex ring, then another with double the number of beads. For example, to make a 7-membered-ring nanocone structure, one would need a ring of 7 and a ring of 14 beads (Figure S3c). By placing the smaller ring inside the larger ring, the structure will find its optimal configuration with minimal manipulation by hand (Figure S3d) (see video in Supporting Information II). Due to the polar nature of magnets, sometimes a component will need to be rotated or flipped to create the desired connection.

Students are given 200 neo magnets to experiment with individually, or in small groups. They are free to choose their method when they are tasked with producing pentagonal and hexagonal nanocone structures (Figures 2d and 2e) using the magnets and observing the angles each one naturally forms. It should become apparent that some techniques are easier than others. Students can then move on to other-membered-ring structures (e.g., 2−11, as shown in Figure 2), before freely attempting any other structures they may be interested in. Photographs can then be taken of the structures they have made.

For a more in-depth investigation, a comparison study can be done with computer simulations. With the photographs of structures they have built themselves out of neo magnets, the

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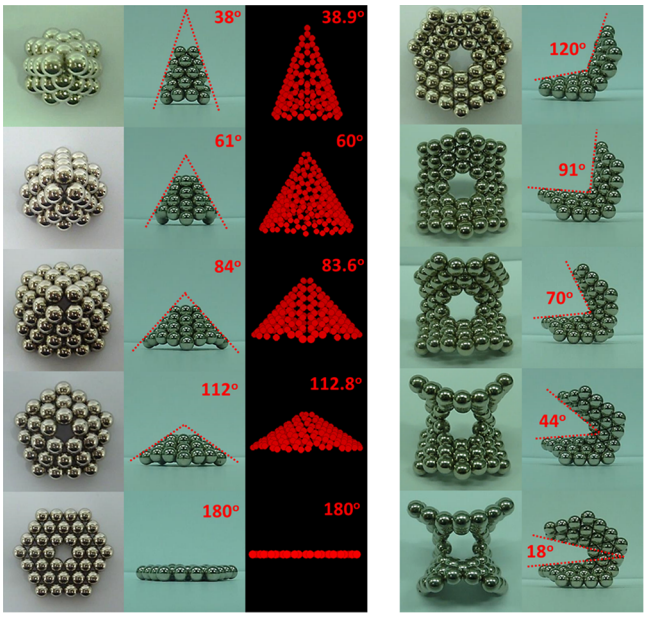

Figure 2. Carbon nanocone structures built with neo magnets, 2−6-membered-ring structures with associated simulations calculated from Nano Modeler (a−e), and 7−11-membered-ring structures (f−j). Angles for individual structures are shown in each inset.

students can measure cone angles from these images. They could compare those to cone angles calculated from structures produced by computer simulation software. The software we have chosen to use was developed by JCrystalSoft, which has many options for constructing different nanostructures.[21] One of the functions allows the user to produce nanocones from graphene sheets. These sheets have predefined disclination angles (for example 60, 90, 120) that represent the sector that is removed from the graphene sheet before it is wrapped into a cone. The disclination angle is directly related to the number of atoms at the apex of the finished cone, as shown in Figure 3. Nanocones with apex rings 2−6 can be calculated with Nanotube Modeler.

To conclude, the students can compare the cone angle difference obtained from both methods and, if there are many groups, check if results are consistent across the groups. A group discussion may be advantageous in the final stages to highlight and reiterate important concepts involved in this activity.

HAZARDS

Due to the magnets' small size and strong magnetism, they can be a swallowing and pinching hazard for younger children; therefore this activity is primarily intended for college students.

DISCUSSION

This activity was trialed on several discussion groups at three different universities, National Tsing Hua University, National Chiao Tung University, and National Hsinchu University of

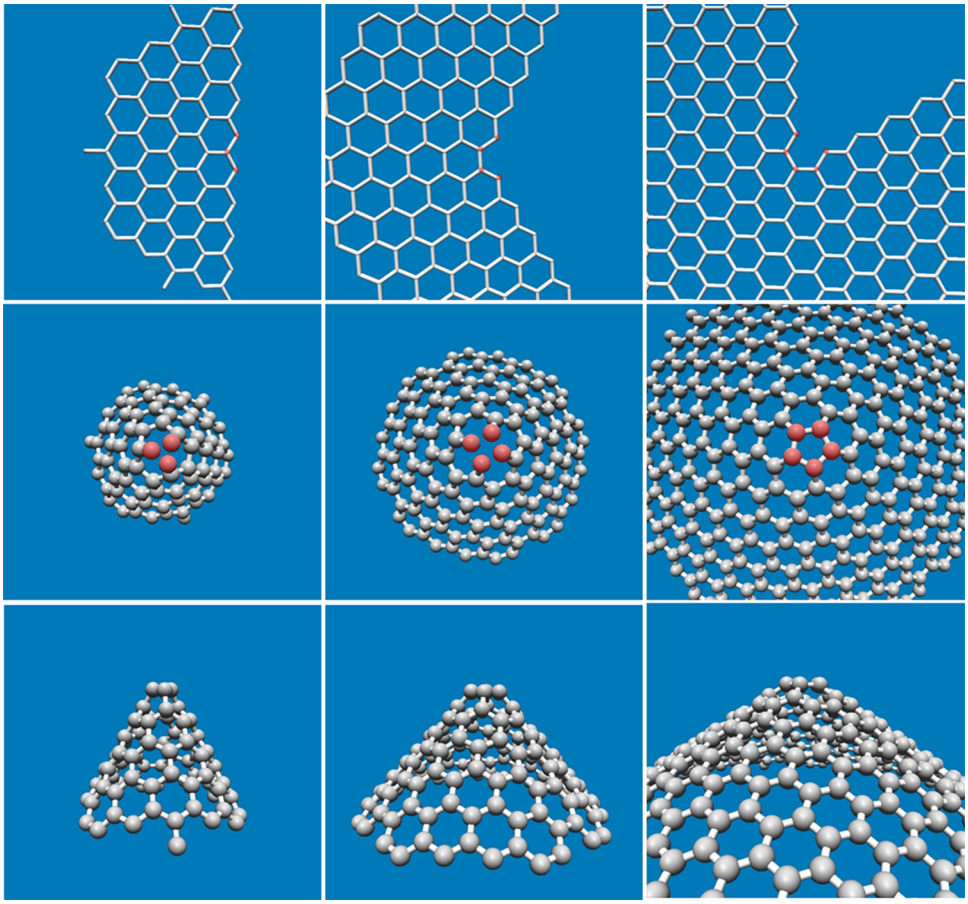

Figure 3. Software-generated images of cone sheets with the predefined disclination angles removed. Highlighted in red are the carbon atoms that become the apex of the nanocone when the sheets are wrapped up. Cone angles are then measured from these calculated structures.

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Education. These groups consisted of approximately 20 undergraduate and postgraduate students from a variety of scientific disciplines such as material science, applied chemistry, and science education. Not only did the activity provoke discussion, students reported gaining a deeper understanding of bonding structure and structure stabilization. Some were even motivated to further explore structures beyond those described within the activity.

In a classroom setting, potential discussion topics can include:

- Stability of each structure and how it relates to its abundance in nature and well-known molecules
- Involvement in larger structures (e.g., nanotubes), with bent "knees" constructed of "defective" pentagons and heptagons
- How defects could affect the shape of the structure

5- and 6-membered carbon rings are no strangers to organic chemistry. Molecules containing such structures are commonplace in biology and naturally occurring substances, in contrast to 3- or 4-membered rings, which are rare. The abundance of 5- and 6-membered carbon rings can be attributed to the stability of these structures, as demonstrated in this activity. Students should have experienced first-hand the strain and difficulty involved in forming the more "unstable" structures, until the magnets find the most stable configuration and click into place. This may help students understand how it is possible for these particular structures to exist and the type of configurations they adopt.

In this activity, structures without defects are made. An interesting topic to discuss could be the effect of defects on these or larger structures that contain defects. Some structures would collapse, while others require defects to take shape. For example, nanotubes are formed from rolled up sheets of graphene made up of 6-membered carbon rings. However, it has been observed that, when a bend occurs in these otherwise straight tubes, the bent "knees" are constructed of 5- and 7-membered rings.[22] These are defects in the graphene structure where the pentagon and heptagon are positioned at two diametrically opposed sides of the structure, allowing the axis of the two connected nanotubes to make an angle of approximately 35°.[22] Understanding how these shapes are formed is crucial to the development of skills in designing nanostructures for potential applications.

Figure 2 shows results from studies we have conducted using the aforementioned software Nanotube Modeler, comparing cone angles from photographs and those from calculations for 2- through 6-membered-ring nanocone structures. The largest angle difference observed between experimental and theoretical values was only 1°, supporting the proposal that neo magnets are a suitable candidate for structural representation of carbon structures. Simulations for the larger structures were not obtained, however the configuration of the 7-membered-ring structure is in concordance with the literature.[23] But the aim of this activity, whether it be a comparison of computer calculated values or data from literature, is for the students to realize that the models in their hands are accurate representations of those nanostructures that cannot be seen with the naked eye.

Technically, each neo magnet does not represent a carbon atom in the nanocone structures shown in Figure 2. In this case, each bead is more appropriately described as the bond between atoms, and the spacing between the beads represents the position of atoms. Thus, the cone angles obtained from photographs are still in concordance with those calculated from computer simulations. We think it is important as educators to point out limitations in the models, or concepts that may be counterintuitive such as the fact that in these neo magnet cone structures the beads do not represent atoms, but bonds between them.

CONCLUSION

This activity proposes an alternative to the traditional modeling medium of ball-and-stick to aid in the 3D visualization of carbon structures, using the popular desktop toy neo magnets. The magnetic beads, held together only by magnetic force, are able to accommodate more angles than those predetermined by ball-and-stick. Students are asked to construct various carbon fullerene structures and are free to get creative. A comparison study with values obtained from computer simulations calculated by Nanotube Modeler was included to further consolidate the understanding of how these structures take shape. Positive feedback was received from trials with university and college students, who reported a deeper understanding of carbon bonding after this fun activity. The exercise aims to give the students a hands-on experience of the importance of specific bond angles for stability as well as an appreciation for the versatility of carbon bonding. This understanding can then contribute to the development of skills in designing new nanostructures for a variety of applications.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.5b00408.

Nanocone structure with apex rings of 6 beads (ZIP)
7-Membered-ring nanocone structure from 7-membered ring inside 14-membered ring (ZIP)
How to build nanocone structures with apex rings of 6 and 7 beads (PDF; DOC)

AUTHOR INFORMATION

Corresponding Author

*E-mail: cylee@mx.nthu.edu.tw.

Notes

The authors declare no competing financial interest.

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