MEGA MOLECULES

Name: ____________________

Date: ____________________

Modeling Activity For The Fullerenes, Buckyball and Carbon Nanotubes

Time required: three 50-minute periods

The Fullerenes

A fullerene is a molecule of carbon in the form of a hollow sphere, ellipsoid, tube, and many other shapes. Spherical fullerenes are called buckyballs, and they resemble the balls used in soccer. Cylindrical ones are called carbon nanotubes .

In this activity, you will use carbon atom models that have an sp^2 hybridization and forms 3 bonds to the neighboring carbon atoms. You might argue that a carbon atom has to form 4 bonds because of its 4 unpaired electrons. These carbon models are a simplification, showing the arrangement of atoms rather than the bonding. Each carbon atom uses three of its electrons to form single bonds to the adjacent carbon atoms. The fourth valence electron is delocalized and free to wander.

Build a Buckyball Model

In 1985 a trio of scientists, Richard Smalley, Robert Curl, and Harry Kroto discovered the buckyball. They vaporized a sample of graphite with an intense pulse of laser light and used a stream of helium gas to carry the vaporized carbon into a mass spectrometer. The mass spectrum showed peaks corresponding to clusters of carbon atoms, with a particularly strong peak corresponding to molecules composed of 60 carbon atoms, C60. The soccer ball shaped C60 molecule in Figure 1 was named “buckerminsterfullerene” or “buckyball” for short. It is a member of a group of similar structures known as the fullerenes.

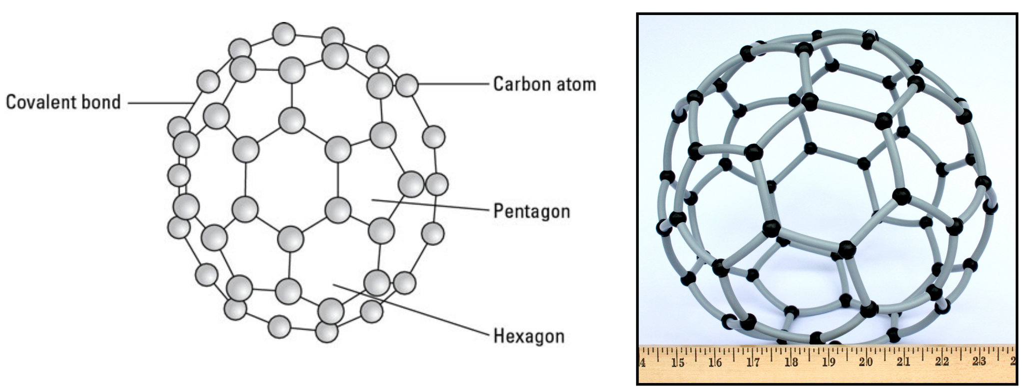


Figure 1

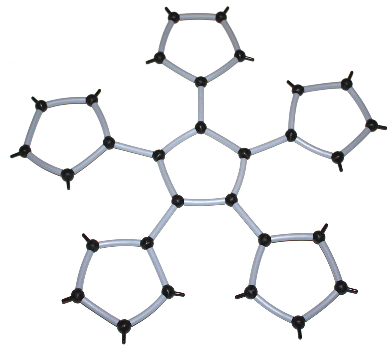
This new allotrope of carbon is spherical in shape with 32 faces, 12 pentagons and 20 hexagons. The buckyball has 90 covalent bonds. Each carbon atom has three valence electrons that are used to form three single covalent bonds, while the remaining valence electron is delocalized over the surface of the spherical molecule. Build the buckyball using 60 sp^2 carbon atom models and 90 single bonds.

Step 1: Build 12 pentagon structures.

Figure 2

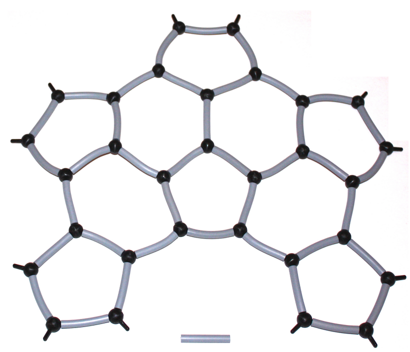
Step 2: Connect 6 of the pentagons together to make 2 of the following structures.

Figure 3



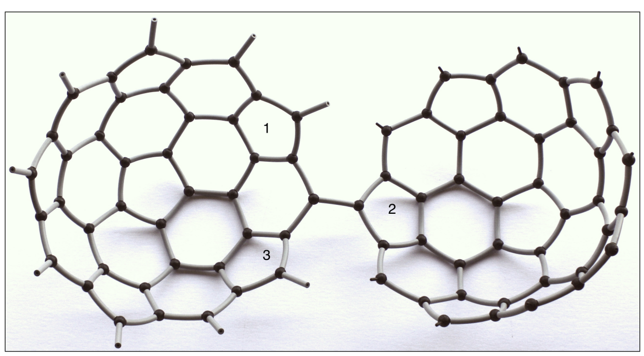
Step 3: For each structure, connect the pentagons together forming 5 hexagons between the pentagons. Once connected, you will have made half of the buckyball.

Figure 4



Step 4: Place pentagon #2 between the pentagons on the opposite half of the buckyball. Connect the halves forming a hexagon. Continue to add the remaining bonds to complete the buckyball model.

Figure 5



Buckyballs have the interesting electrical property of being very good electron acceptors, which means they accept loose electrons from other materials. This feature is useful, for example, in increasing the efficiency of solar cells in transforming sunlight into electricity. Research additional uses of buckyballs.

Build Models of Carbon Nanotubes

A carbon nanotube is a graphene sheet that has been rolled into a tube. Nanotubes are members of the fullerene family, which also includes the spherical buckyballs. The ends of a nanotube might be open or capped with a hemisphere of the buckyball structure. Their name is derived from their size, since the diameter of a nanotube is on the order of a few nanometers which is approximately 1/50,000th of the width of a human hair. There are three unique geometries of carbon nanotubes: zigzag, chiral, and armchair. Carbon nanotubes have novel properties that make them potentially useful in many applications. They exhibit extraordinary strength and unique electrical properties, and are efficient thermal conductors.

The three geometries of carbon nanotubes can be classified by how the graphene sheet is wrapped into a tube and is represented by a pair of indices (n, m). If m = 0, the nanotubes are called zigzag (n, 0). The nanotubes are called armchair (n, n) if n and m are equal. Otherwise, they are called chiral (n, m).

Use Figure 6, sp^2 carbon atom models, and single bonds to build the graphene sheet. Roll the graphene sheet so that carbon (0,0) lines up near carbon (9,0). Connect the bonds to complete the carbon nanotube model. This nanotube has 10 carbon atoms along the top circumference and is named zigzag (10,0). To make a closed-end nanotube, cap the ends with half of the buckyball structure.

Figure 6

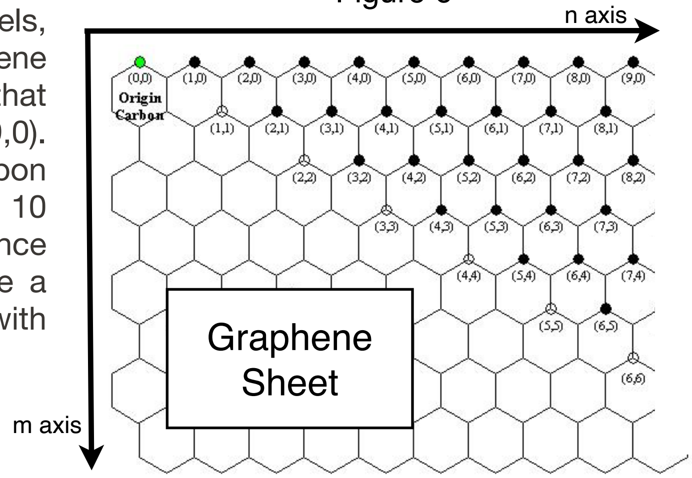
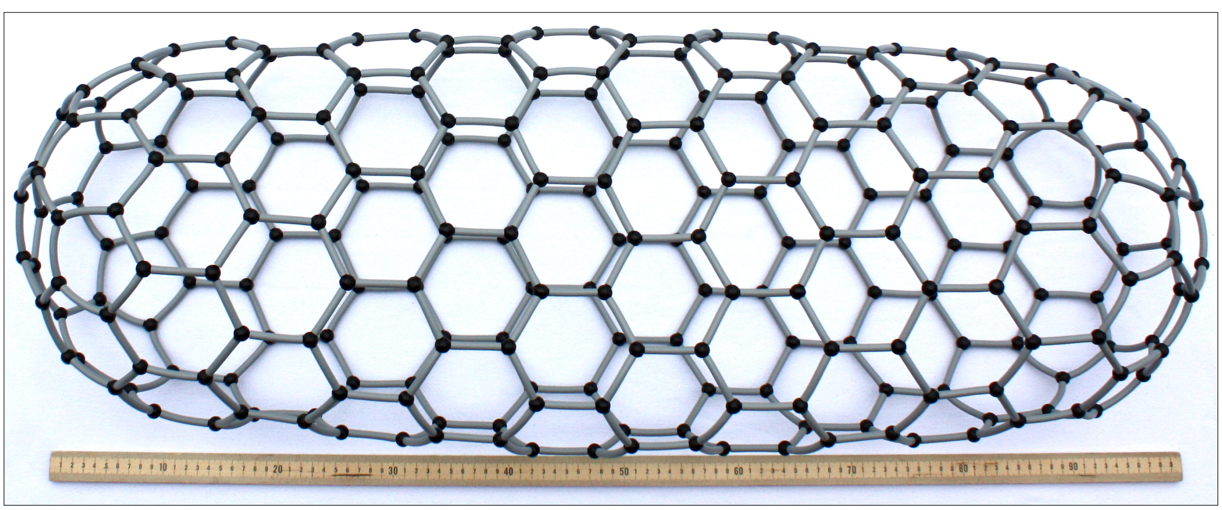


Figure 7
Zigzag Nanotube

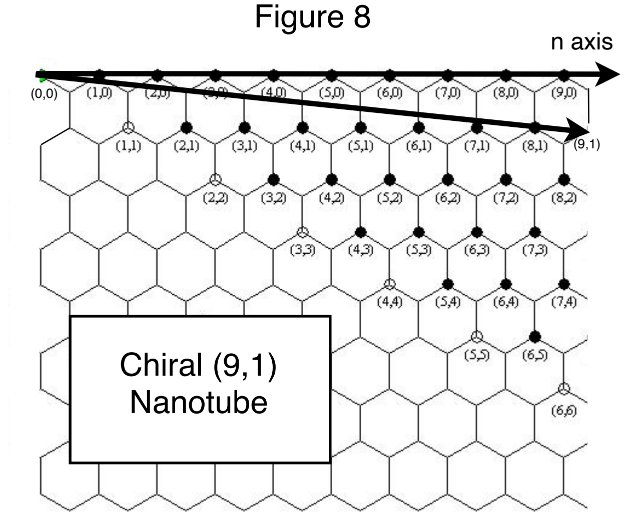


There are many ways to roll a graphene sheet. The way the graphene sheet is rolled up determines the values of n and m and the chirality, or "twist" of the nanotube. The chirality in turn drastically affects the electrical conductance of the nanotube, it's density, it's lattice structure, and other physical properties. For a given (n,m), the nanotube is metallic and an electrical conductor if (2n + m)/3 is an integer. Otherwise it is a semiconductor. The zigzag nanotube (10,0), shown in Figure 7, is a semiconductor.

The chiral angle is the angle between the n axis and the direction in which the graphene sheet is rolled up. The zigzag nanotube has a chiral angle of 0^{o}. The second type of carbon nanotube, the chiral nanotube, has a has a chiral angle greater than 0^{o} and less than 30^{o}.

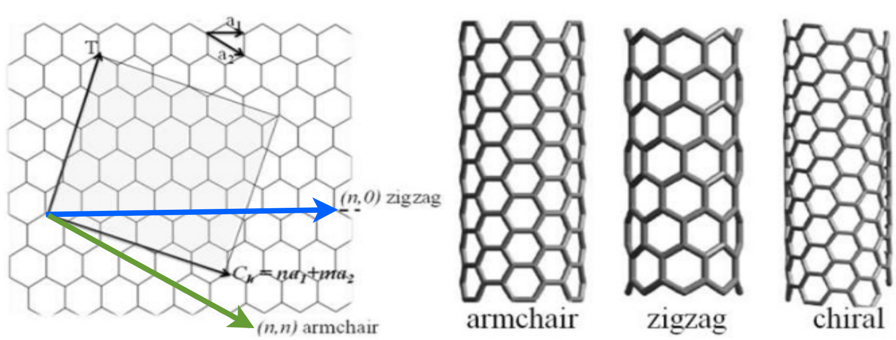
Build the graphene sheet shown in Figure 8. Connect carbon (0,0) to location (9,1). Connect the bonds to complete the carbon nanotube model. Use the equation, (2n + m)/3, where n = 9 and m = 1, to determine whether this chiral nanotube is an electrical conductor or a semiconductor?

Figure 8



If the graphene sheet is rolled in the direction of the green arrow (n,n) shown in Figure 9, the nanotube is armchair geometry. All armchair nanotubes are metallic. Studies have shown that the electrical and magnetic properties of the metallic nanotubes are diameter dependent.

Figure 9



Build the graphene sheet in Figure 10 to construct the armchair carbon nanotube. Roll the graphene sheet along the green arrow. The armchair nanotube has a chiral angle of 30º. Connect the bonds to complete the carbon nanotube model.

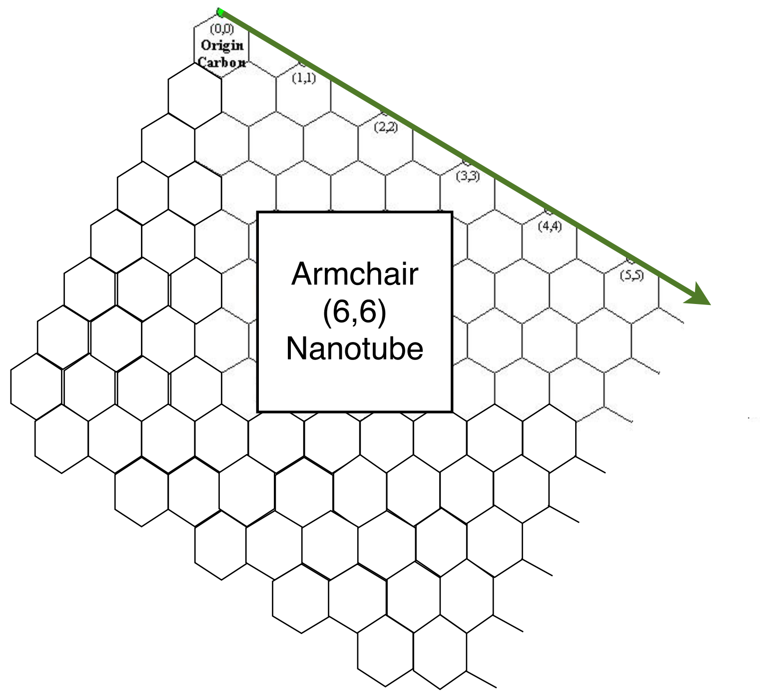


Figure 10

Summary

In this modeling activity you have constructed a buckyball, and carbon nanotubes. What are the three unique geometries of carbon nanotubes?

Carbon nanotube science is relatively new. Scientists from the fields of chemistry, physics, and the material sciences are just beginning to unlock the mysteries and hypothesize about the potential applications of carbon nanotubes. Use the internet to research recently discovered applications for these new materials.