Overview
This activity focuses on the effect of electron repulsions on molecular shape. Both the electron geometries and resulting molecular shapes are discussed with an emphasis on shared and unshared electron pairs as defining factors in the observed shape of a molecule.

Learning Objectives
Students will be able to:
• Explain that the three-dimensional shape of a molecule is dependent on interactions of electrons, including repulsion to other electrons and attraction to nuclei.
• Recognize linear, trigonal planar, and tetrahedral molecule shapes based on areas of electron density.
• Explain how both shared and unshared electrons (as represented in Lewis dot diagrams) influence a molecule’s geometry and use this knowledge to predict the 3D shape of a molecule.
• Differentiate between electron geometry and molecular shape.
• Apply their understanding of small molecule geometry to larger molecules such as fatty acids.

Possible Student Pre/Misconceptions
• Molecules are flat (two-dimensional).
• Large and complicated molecules have simple geometries.
• The electron pairs in atoms are static and do not move once they reach their equilibrium positions.

Models to Highlight and Possible Discussion Questions
After completion of Part 1 of the activity:
Models to Highlight:
• Page 2 – Attractive and Repulsive Forces
  o Review the areas of electron density and the concepts of attractive and repulsive forces. Review structure of an atom. Refer to page 3 from the Atomic Structure activity. Review orbitals and how they relate to electron density.
  o Link to other SAM activities: Electrostatics. Review the idea of like charges repelling and unlike charges attracting.
• Page 4 – Hydrogen Molecule
Link to other SAM activities: **Chemical Bonding.** Review covalent bonds and regions of likely finding electrons.

**Possible Discussion Questions:**

- What are regions of electron density? How does this fit with what you know about the structure of the atom? How does this fit with what you know about chemical bonding? (Focus particularly on differences between polar and non-polar covalent bonding, and ionic bonding.)
- **Demonstration/Laboratory Ideas:** Build molecules using molecular lab kits to correspond with this activity.

**After completion of Part 2 of the activity: Models to Highlight:**

- Page 6 – Electron vs. Molecular Geometry
  - Highlight the importance of both shared and unshared electron pairs. Use the Lewis dot diagram and the 3D model to check understanding of the difference between electron geometry and molecular shape.
- Page 8 – Model of Straight and Kinked Fatty Acid Chains
  - Describe the geometry around various carbon atoms in the chains. Have students apply terms learned earlier in the lesson. Encourage students to zoom in on the molecules and manipulate them to see all electron-dense regions.
- Page 9 – Melting Points of Butter vs. Oil
  - Highlight what happens to each substance as temperature is increased. Remind students that the models are running simultaneously. When does butter melt compared to oil? Why? How is that linked back to their molecular geometry?
  - Link to other SAM activities: **Heat and Temperature, Phase Change.** Take this opportunity to tie into other fundamental concepts that have already been covered.

**Possible Discussion Questions:**

- Why do you think some fatty acids (trans fatty acids) are considered to be bad for your health? How is this related to their molecular geometry?
- What are some examples of molecules that must have a “good molecular fit” in order to work correctly? Where do we see real-world applications of this? (Ideas: drug targets, enzyme/substrate relationship.)
- Why do different materials have different boiling points? How does shape play a role in boiling point? In surface area?
Connections to Other SAM Activities

The focus of this activity is to explore the basic concept behind why molecules have specific three-dimensional structures. It is based on the VSEPR (valence shell electron pair repulsion) theory. Both bonded and unshared electron pairs in molecules repel each other to form the most energy-efficient geometry possible.

This activity is supported by **Electrostatics** where students learn about the basic nature of repulsion of like charges. In **Atomic Structure** students explore an atom’s structure, composed of a core of positive charge (the nucleus) and a shell of negatively charged electrons. In **Chemical Bonds**, bonds are described as regions of electron density between atoms.

**Four Levels of Protein Structure** focuses on protein shape resulting from different types of molecular interactions. In addition, **Protein Partnering and Function** explores how the shape of the molecule itself is essential to its function. In **Lipids and Carbohydrates** and **Nucleic Acids and Proteins** students investigate the relationship between general shapes and functions of these molecules.
Activity Answer Guide

**Page 1:**
*Introduction, no questions*

**Page 2:**
1. Explain why the electrons move to their new positions.

   The electrons must be as far away from each other as possible (repulsion) and still as close to the nucleus as possible (attraction).

2. What keeps electrons from moving away from the atom altogether? Choose the best answer: (c)

**Page 3:**
1. Tetrahedral

2. Linear

3. Trigonal Planar

4. How many regions of electron density are around the central atom in a molecule with tetrahedral geometry? (d)

5. How many regions of electron density are around the central atom in a molecule with linear geometry? (b)

6. How many regions of electron density are around the central atom in a molecule with trigonal planar geometry? (c)

**Page 4:**
Rectangles show areas of electron density.
Page 5:

1. Step 1: Look at the Lewis dot structure for CO$_2$ (above). What is the central atom in CO$_2$? (a)

2. Step 2: How many regions of electron density are there around the central atom in CO$_2$? (b)

3. Step 3: Think about electron repulsions and how regions of electron density arrange themselves around a central atom. Then...

   4. Step 4: Predict the shape of carbon dioxide: (a)

5. Predict the shape of boron trifluoride: (b)

6. Explain why boron trifluoride has the geometry it does:
   There are three regions of electron density around the central atom (boron). These regions will repel each other and result in a trigonal planar geometry.

Page 6:

1. What is the electron geometry of water? Click here to see the steps for determining geometry. (c)

2. Describe how unshared electrons are responsible for the angle of the water molecule.

   The central atom (oxygen) is bound to two hydrogen atoms. However, there are also two sets of unshared electrons that repel each other and result in the bent shape of a water molecule.

3. Carbon dioxide (CO$_2$) and water (H$_2$O) both have two atoms attached to the central atom. Explain why carbon dioxide's shape is linear, while water's shape is bent. (Click here to compare the Lewis structures of CO$_2$ and water.)

   In a carbon dioxide molecule, the central atom (carbon) is only surrounded by two regions of electron density, resulting in a linear shape. These are the two double bond regions that carbon shares with two oxygen atoms.

In a water molecule, the central atom (oxygen) is bound to two hydrogen atoms, but still has two other electron pairs remaining unbonded. These unbonded regions still repel and result in the tetrahedral shape of a water molecule.

Page 7:

1. Make a prediction for the shapes of NH$_3$ and BF$_3$, shown at right: (b)

2. Place your snapshot of NH$_3$ with the added unshared electron pair here:

   Sample snapshot:

   ![NH$_3$ with the unshared electron pair illustrated.](image)

   NH$_3$ with the unshared electron pair illustrated.

3. Explain your placement of the unshared electron pair in the snapshot at left.

   The NH$_3$ has a total of four regions of electron density. The circled area in the snapshot represents the area where an unshared pair is located as a result of being repulsed by the shared electrons. Because there is also a repulsion by the unshared electrons the molecule has a trigonal pyramidal shape and not a planar shape.

4. The shape of NH$_3$ is called "trigonal pyramidal." What is its electron geometry? (c)

5. Explain why the shape of BF$_3$ is the same as its geometry:

   In BF$_3$, there are three bonds surrounding the boron atom and no unshared pairs of electrons to add to the repulsive force.
Page 8:

1. Which numbered atoms have trigonal planar geometry? (e) (f)

2. Which numbered atoms have tetrahedral geometry? (a) (b) (c) (d)

3. Which numbered atoms have trigonal pyramidal geometry? (g)

Page 9:

1. Which of the two solids melts (becomes a liquid) first? (b)

2. Using your knowledge of close range intermolecular forces (van der Waals forces), explain how shape influences the melting points of butter and oil.

The molecules in butter are packed more closely together. There are more intermolecular attractions because of how they align in close proximity to one another. In oil, the particles cannot pack together as closely and, therefore, have fewer intermolecular attractions holding them together. Thus, oil requires an input of less energy to cause it to melt.

Page 10:

There are many fascinating uses for nanotechnology. Use one of the links below to search for an interesting example on the Web, or to find your own. When you find one that is compelling to you, paste the URL of the page below, and explain how nanotechnology is put to work in your example.

Answers will vary.

Page 11:

1. The position of the electrons around an atom is NOT a result of: (c)

2. Which of the following are regions of electron density? (Check all that apply.) (a) (b) (d)

3. Do electron dot structures accurately describe the shapes of molecules? Explain your answer.

No. They show the bonds and unpaired electrons. However, they do not show the three-dimensionality of the atoms relative to one another. The positions of the atoms are a result of the repulsive force of the electrons.

4. Below is the Lewis structure for phosphorus trichloride. Choose the correct molecular geometry from the list below. (e)

5. Is the shape of xenon trioxide the same as its electron geometry? Explain why or why not.

No. Its electron geometry is tetrahedral and due to the unshared electron pair, its shape is trigonal pyramidal.

6. Predict the electron geometry of nitrosyl chloride, shown below. (c)

7. In the previous question, you were asked to predict the electron geometry of nitrosyl chloride. Now, predict its shape and explain your answer:

There are three regions of electron density around the central atom: one pair of electrons that is unshared and two pairs that are shared in the two bonds. So, since all three regions are repelling each other, the geometry is trigonal planar. But because only two regions connect to atoms, the molecule appears bent.

8. Explain how molecular shape plays a role in determining the temperature at which a solid melts into a liquid.

The shape of a molecule determines how much attraction there is between its atoms. These are known as van der Waals forces. As seen in the model on page 9, when molecules are packed closely together, there is more attraction and it is harder to pull them apart. That is, it would take a higher temperature to make them melt. When molecules are more loosely packed, there are fewer intermolecular attractions, which would allow them to melt into a liquid and lose their solid structure more easily (at lower temperatures).
SAM HOMEWORK QUESTIONS
Molecular Geometry

Directions: After completing the unit, answer the following questions to review.

1. The shape of a molecule allows it to do its job. The interaction of electrons determines that shape. In the picture shown below, use arrows to draw in both the attractive and repulsive forces.

2. For each of the pictures below, label the molecular shape as one of the following: linear, trigonal planar, or tetrahedral.

3. The electrons that surround atoms determine molecular shape. Is it the shared electrons, unshared electrons, or both that affect how a molecule will look in 3D? Explain your answer.

4. What is the difference between saturated and unsaturated fats? First, answer this question on the macroscopic scale. (What is different in how they look at room temperature?) Then, answer the question at the atomic scale. (What is different about how the atoms are arranged?)

5. Why might it be advantageous to be able to predict the 3D shape of a molecule? Give a specific example to support your answer.

6. How many regions of electron density surround carbon (grey atom) in the diagram to the left? _____

What is the shape of the molecule that is formed? ______________

7. Career connection: One of the most important problems scientists are trying to solve is how to predict the shape of protein molecules produced by the genes in our cells. Check out the Folding at Home project - http://folding.stanford.edu/ - and describe why this is important. (You can install free modeling software to help them work on protein folding.)
SAM HOMEWORK QUESTIONS
Molecular Geometry – With Suggested Answers for Teachers

1. The shape of a molecule allows it to do its job. The interaction of electrons determines that shape. In the picture shown below, use arrows to draw in both the attractive and repulsive forces. Electrons are attracted to the nucleus and repel each other. See similar image.

2. For each of the pictures below, label the molecular shape as one of the following: linear, trigonal planar, or tetrahedral.

3. The electrons that surround atoms determine molecular shape. Is it the shared electrons, unshared electrons, or both that affect how a molecule will look in 3D? Explain your answer. Both. It is the number of regions of electron density around a central atom that determines molecular shape. For molecules with no unshared pairs of electrons around the central atom the geometry and the shape are exactly the same. When a molecule has unshared electrons around its central atom, its shape can be different than its geometry.

4. What is the difference between saturated and unsaturated fats? First, answer this question on the macroscopic scale. (What is different in how they look at room temperature?) Then, answer the question at the atomic scale. (What is different about how the atoms are arranged?) Saturated fats, such as butter, are usually hard solids at room temperature while unsaturated fats, such as oil, are usually liquid. On the atomic scale, saturated fats have bonded with as many hydrogen atoms as they can accommodate and are considered a straight chain fatty acid whose components can line up tightly next to one another. Unsaturated fats have a kinked chain. The kink prevents as close of an association, resulting in a liquid at room temperature.

5. Why might it be advantageous to be able to predict the 3D shape of a molecule? Give a specific example to support your answer. To predict how a molecule will behave or interact with another molecule. Examples could include drug design or nanomachines.

6. How many regions of electron density surround carbon in the diagram to the left? __2__

What is the shape of the molecule that is formed? Linear

7. Career connection: The nature of many genetic diseases is related to the form and function of proteins. By understanding how proteins fold new drugs could be developed and provide a better understanding of how living things function.