Drexel University – NanoEnlightenment

Self Assembly Lab

Background
While one of the promises of nanotechnology is the development of customized nanodevices, there are significant challenges associated with manipulation of the extremely small sized nanoparticles. One area scientists are exploring to enable custom designed devices is self assembly. Self assembly involves dumping customized nanoparticles together that spontaneously assemble themselves into the desired structure. (Imagine dumping jigsaw pieces in a box and a puzzle is spontaneously produced).

We can find many examples of self assembly in nature including the assembly of water molecules into snowflakes, cells combining to form tissues, bones and organs or the formation of sea shells. A simple example of self assembly is the spontaneous formation of a covalent bond between 2 atoms and at its most elegant, the formation of the DNA double helix.

Self assembly can involve intermolecular or intramolecular assembly. If you studied chemistry, you are familiar with simple intermolecular assembly since any 2 or more materials that spontaneously combine without human physical manipulation could be considered self assembly. For example under certain circumstances, carbon dioxide can be made to react with hydrogen gas to produce methane and water vapor. The formula for the reaction is:

$$\text{CO}_2 + 4\text{H}_2 \rightarrow \text{CH}_4 + 2\text{H}_2\text{O}$$

The formation of the bond between carbon and hydrogen to produce methane involves self assembly. The results are predictable. If the conditions are favorable for the reaction to occur you always end up with exactly the same methane molecule, always 4 H atoms to 1 carbon atom and always with carbon in the center.

A good example of intramolecular self assembly is protein folding. Proteins are long chains of amino acids. For a protein to function correctly it must not only have the correct sequence of amino acids but it must also fold into the proper 3 dimensional shape. If proteins don’t fold correctly, diseases can result. Diseases associated with misfolding include Alzheimer's disease, cystic fibrosis, BSE (Mad Cow disease), an inherited form of emphysema, and even many cancers. http://folding.stanford.edu/science.html

In both intermolecular and intramolecular assembly, what determines if self assembly will occur and into what structure are shakiness and stickiness. http://www.physics.unc.edu/classes/fall2005/phys006d003/Lego_Self_Assembly_Pamphlet_Final.pdf

Shakiness can be considered the energy factor or temperature. You must be at the right temperature for the assembly to occur. Energy must be high enough to bring particles in
close enough contact to bond but not so high as to break desired bonds. Stickiness can be considered attractive forces and geometry. Particles must have attractive forces that bring them together and their shapes must be such that they are allowed to physically come together. The attractive forces all come about from differences in charge, with strongest forces being intramolecular ionic bonds to the weakest forces being intermolecular Van der Waal forces or hydrophobic bonding. 

http://www.physics.unc.edu/~falvo/Phys006D_Fall06/Lectures_PPT/4_STICKINESS_Fall_2004.ppt

Much of the research being done on self assembly involves attempts to understand biological models of self assembly as a template for how nano machines could be produced. This area of study is in its infancy and the challenges of modeling, let’s say protein folding, are enormously complex. A model of a protein folding can be found at http://intro.bio.umb.edu/111-112/111F98Lect/folding.html

We will start more simply by observing how simple materials self assemble. In this lab you will simulate both intermolecular and intramolecular self assembly. While self assembly in the real world occurs in 3 dimensions, we will simplify things by working in 2 dimensions.

Materials:
- Bag containing Styrofoam cutouts including:
  - 20 white foam circles, 20 orange triangles and 20 yellow squares and
  - 12 2 sided orange/blue foam circles.
  - 10 ¼” by 1/16” magnets
  - 20 1/8” by 1/16” magnets
- Rectangular bucket (like plastic storage containers) at least 6 inches by 12 inches and 2 inches deep.
- Water to fill bucket to ½”
- Digital camera
- Glue gun and several glue sticks
- Thin cotton string (thicker than thread)

Part 1
1) Fill the bucket with about ½ inch of water.
2) Drop 10 of the white circles into the water so they float on the water and do not lie on each other.
3) Observe the circles undisturbed for 5-6 minutes and record your observations in results section 1.
4) For 2-3 minutes tap or sway the bucket (without putting your hands inside), in effect changing shakiness in an attempt to increase self assembly. Make sure to try both gentle and vigorous movements. Record your observations in results part 1 and answer questions.

5) Remove the white circles and repeat steps 2 then 4 with the orange triangles and then repeat steps 2 then 4 with yellow squares. Record your observations and answer questions in results section 1

Results Part 1 Impact of Shakiness and Shape

Circles:
Include a photograph of what the circles looked like when you first dropped them on to the water here:

Include a photograph or draw a diagram of what the circles looked like after 5-6 minutes on the water surface undisturbed.
Include a photograph or draw a diagram of what the circles looked like after 2-3 minutes of manually varying the energy in the container.

Include a photograph or draw a diagram of what the squares looked like after 2-3 minutes of manually varying the energy in the container.

Include a photograph or draw a diagram of what the triangles looked like after 2-3 minutes of manually varying the energy in the container.

**Part 1 Questions:**
1) Did any of the circles self assemble without the aid of tapping or swaying?

2) What do you think caused this self assembly to occur?

3) Did adding energy to the container increase the rate of self assembly?

4) If so, why was the rate of self assembly increased when you increased energy?

5) What happened when you added too much energy? Too little energy?

6) What differences if any did you observe with the self assembly of the triangles or rectangles vs. the circles?

**Part 2: Impact of stickiness**
1. Fill the bucket 1/2” or so with water.
2. Drop all of your 2 sided orange/blue foam circles onto the water with the same color facing up. All of the 2 sided orange/blue foam circles have a magnet sandwiched inside with the polarity in the same direction. When all the same color is facing up their polarity is the same. For the sake of consistency you could say the orange side is - and the blue side is +.
3. Give the circles a couple of minutes to self arrange. Record your observations below.
4. Now turn half of the circles over so half are blue and half are orange and let some self assembly occur for a few minutes. You can provide some energy or reach in to remove circles from the sides. Record your results below.

Results – Part 2 stickiness
1. Include a picture here of what the arrangement looks like with all the same color facing up?

2. Explain what is causing this arrangement.(repulsive forces of like charges).

3. Include a picture here of what the arrangement looks like with both orange and blue facing up.

4. Explain what happens when you allow these circles to self assemble and why.

Part 3: Self assemble a molecule
Using what you learned in part 1 and 2, self assemble a molecule. It could be as simple as H₂O or as complex as a benzene ring.

1) Chose shapes/colors specific to each atom involved.
2) If you want to use magnets in the foam, you should attach a magnet to the center of the foam shape and then glue a similarly shaped foam piece on top, aligning edges. This should be done with a glue gun. By sandwiching the magnet between the 2 pieces of foam, you avoid the problem of the magnets being pulled off the foam by the attractive force of adjacent magnets.
3) This may require some trial and error regarding shape selection, magnet size and magnet placement.
4) You are likely to encounter challenges with shapes sticking to the side of the container. You are allowed to put your finger in and gently move the pieces from the edge.
5) Your results are not likely to be perfect. If you get the desired shape 50% of the time or most of the shape correct most of the time, you are doing well.

Results: Part 3
Include a photograph or draw a diagram of the self assembled molecule. Be sure to label which shapes represent which atoms.

1) What challenges did you face with self assembling your molecule?

2) Explain how shakiness and stickiness helped or hindered your molecule self assembly.

Part 4: Fold a protein
Go to this link [http://folding.stanford.edu/education/protein.html](http://folding.stanford.edu/education/protein.html) and read about proteins, specifically peptides. You will make a polypeptide chain using 19 white circles and string. You will then add R groups (see peptide descriptions) limited to those that are polar (either + or -), in select locations on the peptide chain. Not all peptides will have an R group side chain. Your placement of the R group side chains should be determined so that when the chain is placed in the bucket of water the chain will self assemble into a predetermined shape.
1) Make a peptide chain
   a. Make a chain of 19 evenly spaced white foam circles by using a glue gun to attach a string to them. (use 2 cm circles with 1 cm spacing between circles).

2) Add polar side chains to select sites on the peptide.
   a. Use the 2 sided orange/blue disks. Sandwiched between the disks are rare earth magnets. Use a glue gun to attach them to select peptide locations. The blue side can be considered positive polarity and the orange side can be considered negative polarity.

3) Add shakiness
   a. Layout the protein chain as shown above in the water making sure the disks are turned up to the desired polarity/location.
   b. Add shakiness “energy” to the system by tapping the container or moving it from side to side.
   c. You may need to reach into the water to remove circles from sticking to the edges.

4) Modify your polar side chains on the peptide and until you get the desired folded chain structure.

5) Define your polymer structure
   a. You can find information about amino acids and a table of them here: [http://folding.stanford.edu/education/AminAcid.html](http://folding.stanford.edu/education/AminAcid.html) Go take a look.
b. Using the table of amino acids select a sequence of amino acids that could represent the successful polymer you designed. Peptide locations without side chains should be considered those with no or neutral R side chains. Blue disks should be an amino acid that has a positively polar R side chain and orange disks should have negatively polar R side chains.

c. The sample protein shown above could have the following amino acid sequence

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Part 4 Make a Strand of DNA

Using everything you’ve learned here make a strand of DNA using self assembly.

Results: Part 4 DNA

1. Include pictures here. Be sure to label what is in the DNA structure in your pictures.

2. Write a procedure for how you made the DNA.

References:
http://mrsec.wisc.edu/Edetc/