

# Molecular Self-Assembly

ERIC ROSENBAUM

## Teacher Guide

**Biology:** Molecular Biology

**CD:** Molecular Workbench – Self-Assembly

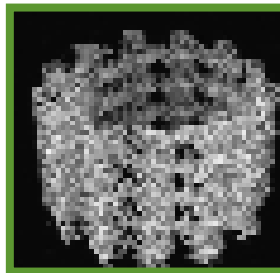
**Web:** [www.concord.org/resources](http://www.concord.org/resources)

**Grades:** 9-14

**Imagine this:** You dump a pile of Lego pieces on the floor, and they start bouncing around, sometimes snapping together. Gradually, elaborate Lego structures form: bridges, buildings, vehicles, and even little machines that take apart and put together other little machines. All this happens without any human intervention.

It sounds like magic, but something very much like this is constantly occurring at the molecular scale in every cell in your body. Called self-assembly, it's the spontaneous formation of ordered structures from smaller parts. Lipid bi-layers form this way, as do many biological macromolecules, such as enzymes made up of multiple polypeptide chains. Protein folding is a type of self-assembly, and so is crystal formation. In these examples, order emerges from disorder, and although the process seems mysterious, a few basic principles of molecular motion and attraction can help explain it.

The *Molecular Logic* project has developed an activity for secondary and college-level students to learn about self-assembly. It's one of a sequence of activities developed



**Figure 1:** A segment of a microtubule. Microtubules are polymers made of many tubulin monomers.

by the Concord Consortium that uses dynamic models to help students reason about biology at the molecular scale.

## Launching the activity

To view the self-assembly activity, open Molecular Workbench – Self-Assembly on the CD, or point your web browser to:

<http://molo.concord.org/database/activities/231.html>

When you click the “launch activity” link, the Molecular Workbench software will automatically download (approximately 4MB), and display the first page of the activity.

*Note:* Molecular Workbench runs on Windows, OSX, and Linux. If you're having trouble running the activity, you may need to download the latest version of *Java*.

## How does self-assembly work?

The activity begins by introducing the two key factors on which self-assembly depends: motion and stickiness.

Motion is the random jostling of all molecules due to their heat energy. For two molecules to “stick” to each other, they need to be close together and lined up in the right orientation. Thermal motion guarantees this will happen eventually.

“Stickiness” refers to intermolecular attractions, those weak forces that make molecules stick to each other, from the small van der Waal's force to the stronger hydrogen bonds and Coulomb forces. While these forces may be weak individually, together they can add up to a strong attractive force between two molecules that are shaped just right to fit together.

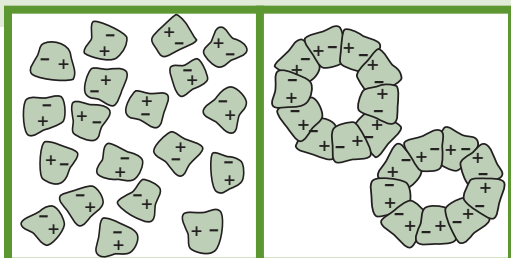
So, with thermal motion jostling molecules around and intermolecular attractions to make them stick, spontaneous structures can start to form.

## Molecular Logic Database

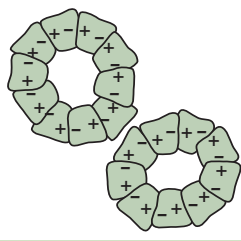
The *Molecular Logic* project seeks to improve the ability of students to understand fundamental biological phenomena in terms of the interactions of atoms and molecules. To view the Molecular Logic Database of over 100 activities, go to:

<http://molo.concord.org/database/browse/stepping-stones/>

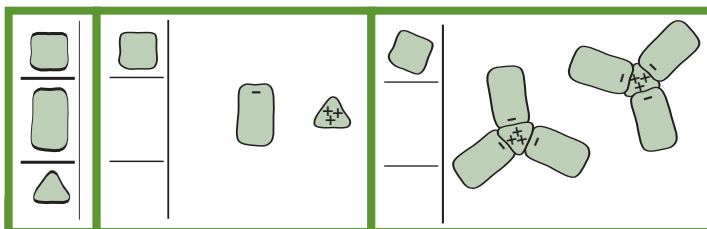
Here you will find, among others, activities that cover life's macromolecules, intermolecular attractions, protein synthesis, and protein folding.



**Figure 2: Self-assembling rings: before (left).** Wedge-shaped monomers, with positive and negative charges, start out in disarray.



**Figure 3: Self-assembling rings: after (right).** Opposite charges attract, and the wedges assemble into a stable configuration.



**Figure 4: Three different monomer shapes (left).**

**Figure 5: Applying charges to the surface (center).**

**Figure 6: After making copies, students run the model to see new structures assemble (right).**

## Microtubules and self-assembling rings

This activity introduces students to three examples of self-assembling biomolecules: dimers, fibers, and microtubules. An image or interactive 3D model shows the structure of the biomolecule in each case, and is followed by a simplified 2D dynamic model that demonstrates how the structure can self-assemble. Finally, students are challenged to modify the model so that it assembles differently.

Microtubules are long molecular-scale tubes made up of thousands of tubulin monomers (figure 1). They play several important roles in the cell, such as providing structure to the cytoskeleton and acting as molecular conveyor belts. The 2D dynamic model shows the self-assembly of a ring structure, representing a cross-section through a cylindrical microtubule. The model starts with a random array of wedge-shaped monomers, each with a positive charge on one side and a negative charge on the other (figure 2). When students run the model, the wedges gradually assemble into a stable ring formation (figure 3). The challenge asks students to modify the charges on some monomers, and then run the model to see the effect of their changes.

### Make your own molecule

On the final page of the activity, students are presented with a more open-

ended challenge. They are given a set of three different monomer shapes with which to work (figure 4). They choose from these, apply positive and negative charges around their edges (figure 5), and make several copies. Next they run the model and watch how their monomers assemble (figure 6). Students can attempt to create one of several example shapes shown on the page or invent their own. When they are finished, Molecular Workbench creates a printable activity report containing students' answers to the embedded assessment questions, along with any snapshots of models students may have taken.

### Self-assembly and beyond

Self-assembly is not part of the traditional biology curriculum, but it is a powerful idea related to many concepts that are taught. For example, this activity can serve as an engaging introduction to protein folding. With a teacher's guidance, students should be able to generalize from these simple examples to the formation of more complex molecular structures.

After completing this activity students might also be interested in the story of the T4 phage, a virus with a beautiful self-assembling icosahedral capsid. The virus contains a small amount of genetic material, which seems hardly enough to contain the instructions for building its complex, symmetrical shell made of thousands of parts. It turns out that these parts are identical monomers that self-assemble.

Another interesting question for class discussion is whether or not *everything* biological is constructed through self-assembly. You can point out that chemical reactions catalyzed by enzymes are required to form the covalent bonds that hold many structures together. These bonds are much stronger than the charge attractions students see in the self-assembly activity. You can also describe the roles of template-based synthesis (making one nucleotide strand by copying it from another) and chaperone molecules, which push and pull and protect a protein as it folds.

In all these cases, one key principle applies: there is no industrious toddler snapping together all the Lego pieces. These processes are all part of a complex system that, amazingly, organizes itself.

#### LINKS *Friday's Lesson*



**Molecular Logic**

<http://molo.concord.org>



**Java**

<http://www.java.com>

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