Molecular Workbench as a Tool for Blended Learning Courses

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Realizing the Promise of Education Technology

• A nonprofit educational research and development organization based in Concord, Massachusetts.

• We create interactive materials that leverage the power of information technologies.

• Our goal is to improve learning opportunities for ALL students.
Benefits of Blended Model

- Better use of student time outside of class.
- More flexibility for using in-class time.
- Materials should be engaging, motivating, and "deep" (i.e. challenging)
Most of the matter you find around you is in one of three phases: solid, liquid, or gas. A solid holds its shape and does not flow. The molecules in a solid vibrate in place, but on average, don’t move far from their places. A liquid holds its volume, but does not hold its shape — it flows. The molecules in a liquid are about as close together as they are in a solid, but have enough energy to exchange positions with their neighbors. Liquids flow because the molecules can move around. A gas flows like a liquid, but can also expand or contract to fill a container. A gas does not hold its volume. The molecules in a gas have enough energy to completely break away from each other and are much farther apart than molecules in a liquid or solid.

When they are close together, molecules are attracted through intermolecular forces. These intermolecular forces have different strengths for different molecules. The strength of the intermolecular forces determines whether matter exists as a solid, liquid, or gas at any given temperature.

Within all matter there is a constant competition between temperature and intermolecular forces. The kinetic energy from temperature tends to push molecules apart. When temperature wins the competition, molecules fly apart and you have a gas. The intermolecular forces tend to bring molecules together. When intermolecular forces win the competition, molecules clump tightly together and you have a solid. Liquid is somewhere in the middle. Molecules in a liquid are not stuck firmly together, but they cannot escape and fly away either.

Iron is a solid at room temperature. Water is a liquid at room temperature. This tells you that the intermolecular forces between iron atoms are stronger than those between water molecules. In fact, iron is used for building things because it is strong. The strength of solid iron is another effect of the strong intermolecular forces between iron atoms.

As the temperature changes, the balance between temperature and intermolecular forces changes. At temperatures below 0°C, the intermolecular forces in water are strong enough to overcome temperature and water becomes solid (ice).
• Dynamic nature of atomic/molecular systems not easily conveyed with text and static images.

• Animations help, but don’t allow students to construct knowledge. Student is passive learner.

• Models which are computed in real-time allow users to probe the simulation by changing parameters. Student becomes an active learner.

- Open-source cross-platform molecular dynamic engine.
- Calculates complex real-time interactions between atoms and molecules.
- User friendly interface for creating custom model-based activities.
A concise summary of the last 100 years of science is that atoms and molecules are 85% of physics, 100% of chemistry and 90% of modern molecular biology.

–Leon Lederman
... all things are made of atoms — little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another.

– Richard Feynman
The Modeling Environment

- 2D and 3D Molecular Dynamics Models
- 3D Exploration of Static Molecular Representation
- Flash based models
- Quantum physics - tunneling, bonding, time dependent Schrodinger representations
- Abstract dynamic models of DNA, RNA and proteins
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Dynamic Phase Change Model
Other Reasons to Like Models

- Help to provide a concrete scaffold for new abstract concepts.
- Can be used in guided inquiry mode.
- Promotes reasoning and supporting ideas with evidence.
When the model is stopped, you can drag the mouse over one or more molecules to highlight them.
Biology - DNA to Proteins
Follow these steps:
1. Add some atoms (press multiple times to add more):
   - add 2
   - add 10
2. Run ▶ the model.
3. Reset ⏹️ the model and try a different concentration.

Gauge the reaction speed by using the graph to see when the reaction reaches 80% completion.
Chem/Bio - Intermolecular Attractions

Oil and Water Shaken Up and Mixed

press run to see the mixture "settle"

Antibody/Antigen
Modeling Macro-level Systems
the electron transport chain
Quantum Chemistry - Polar Bonds
What is true of the rate at which molecules move into and out of the cell at equilibrium?

- A. More move into the cell than out of it.
- B. More move out of the cell than into it.
- C. Equal amounts move into and out of the cell.
- D. They move randomly, so it is not predictable.
Cells generally stay in equilibrium with their surroundings. What are two ways you know the cell has reached equilibrium?

- A. Water stops flowing into and out of the cell.
- B. The concentrations inside and outside of the cell are the same.
- C. The osmotic pressure inside and outside of the cell is the same.
- D. The cell gets as small as it possibly can.

Check Answer
Describe how the chemical energy in ATP is converted into electric potential energy. (hint)
Set up the model so that it is **IN** equilibrium. Then use the "snapshot" button below the model to take a picture of your setup. Use the "open" button below to place that image here.

Click the Open Button, and then drag a thumbnail here.
The arrow shows that the ball is at its peak, not having any particular direction. As shown by the white color the ball has little (low) kinetic energy.
Previewing Models and
Using a Portal

RITES

Welcome Anonymous User.  LOGIN  |  SIGN UP

PROJECT SIGN IN
Username
Password
☐ Stay Logged In

First Time Here?
Sign up for access as:
Student »
Teacher »

Just want to Try the Units?
View our unit Previews »

IMPORTANT! Before running our software and activities, please view our Technical Notes and Requirements section
“It can be difficult to visualize some of the more complex concepts of chemistry, so the visual models can really help [me] understand these concepts.”
“The best part of using the SAM tools was to be able to see things that we would not normally be able to see with labs. The tools were fun and easy to use, the instructions were straightforward and I found it interesting to watch the simulations.”
In a lesson on electrostatics (not the RI-TEST model) a student referred back to something he had learned while doing a RI-TEST activity. The classroom discussion went far more smoothly as a result of the students having learned about atomic structure via the interactive models.
“Students begging to do more units on the computer ... [and] ... writing more than they usually do in response to something they did only moments before.”
Next Generation Molecular Workbench

Atoms. In Your Browser.
Now you can use our award-winning molecular simulations anytime, anywhere.
Possible Modes of Usage and Best Practices

- During class (full activity or in “projector mode”).
- Outside of class
- Through one of our portals or via MW directly.
- Via a hyperlink embedded in course.
- Individual models embedded into course materials
Customization

- Using MW as standalone app.
- Customizing Portal based activity.

- NSDL grant will help pull together disparate resources.
- Parallel work on Next Gen MW will focus around making customized versions of models and activities.
Finding Models and Activities - Current and Past Projects

- Science of Atoms and Molecules (SAM/RI-TEST)
- High Adventure Science
- Geniverse
- Evolution Readiness
- Electron Technologies
- Innovative Technology in Science Inquiry (ITSI-SU)
- Engineering Energy Efficiency
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Geniverse
Convection
Inquiry Is Key

- Going deeper can simplify science
  - Most scientific phenomena can be explained by fundamental ideas of the atomic nature of matter, conservation of energy, Nature’s tendency toward equilibrium.
  - Science through this lens is more connected - less individual facts to “memorize”.

- Conceptual understanding is the goal.

- Utilize interactive models, to allow inquiry at the atomic level.

- Teachers are essential for inquiry approach to work.
Finding Materials

- Concord Consortium Activity Finder
  http://www.concord.org/activities

- Molecular Workbench Application and Database
  http://mw.concord.org

- Various Project portals
  http://www.concord.org/projects
Contact Info

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subscribe to our newsletter
<table>
<thead>
<tr>
<th>Motion and Energy</th>
<th>Physics</th>
<th>Chemistry</th>
<th>Biology</th>
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<td>Diffusion, Osmosis, and Active Transport</td>
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<td>Heat and Temperature</td>
<td>Gas Laws</td>
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<td>Intermolecular Attractions</td>
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<td>Photosynthesis</td>
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# MCI Results

## Cohort 1 - Chem

<table>
<thead>
<tr>
<th>Group</th>
<th>Pre-test mean</th>
<th>Post-test mean</th>
<th>n</th>
<th>p-value based on paired t-test</th>
<th>Cohen’s d</th>
<th>Effect size</th>
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</thead>
<tbody>
<tr>
<td>Chemistry</td>
<td>39%</td>
<td>47%</td>
<td>348</td>
<td>7.8e-32</td>
<td>0.6</td>
<td>Moderate</td>
</tr>
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Score increases related to number of SAM activities completed

1. MCI gain vs. # of physics activities run (cohort 2 - year 2)
2. MCI gain vs. # of chemistry activities run (cohort 2 - year 2)
3. MCI gain vs. # of bio activities run (cohort 2 - year 2)
## Improvements Over Time

<table>
<thead>
<tr>
<th>Cohort 2</th>
<th>Pre-test mean</th>
<th>Post-test mean</th>
<th>gain</th>
<th>p</th>
<th>d</th>
<th>Effect size</th>
</tr>
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<tr>
<td><strong>Year 1 - Phys.</strong></td>
<td>40%</td>
<td>43%</td>
<td>3%</td>
<td>7.6 e-6</td>
<td>0.2</td>
<td>Small</td>
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<tr>
<td><strong>Year 2 - Phys.</strong></td>
<td>33%</td>
<td>47%</td>
<td>15%</td>
<td>3.1 e-20</td>
<td>1.1</td>
<td>Large</td>
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<tr>
<td><strong>Year 1 - Chem.</strong></td>
<td>45%</td>
<td>51%</td>
<td>6%</td>
<td>8.5 e-16</td>
<td>0.4</td>
<td>Small</td>
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<tr>
<td><strong>Year 2 - Chem.</strong></td>
<td>47%</td>
<td>55%</td>
<td>8%</td>
<td>1.1 e-38</td>
<td>0.50</td>
<td>Moderate</td>
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<tr>
<td><strong>Year 1 - Bio.</strong></td>
<td>30%</td>
<td>33%</td>
<td>4%</td>
<td>2.6 e-07</td>
<td>0.3</td>
<td>Small</td>
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<tr>
<td><strong>Year 2 - Bio.</strong></td>
<td>28%</td>
<td>34%</td>
<td>6%</td>
<td>3.7 e-08</td>
<td>0.5</td>
<td>Moderate</td>
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