



The Concord
Consortium

Molecular Workbench as a Tool for Blended Learning Courses

Dan Damelin, The Concord Consortium
ddamelin@concord.org



The development of this program was funded by the National Science Foundation. Any opinions, findings, and conclusions or recommendations expressed in the materials associated with this program are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

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)

Static attempt at teaching phase change

The phases of matter

solid, liquid, and gas

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.

Intermolecular forces

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.

Temperature vs. intermolecular forces

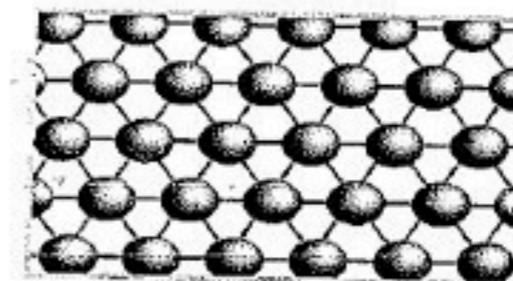
Within all matter there is a constant competition between temperature and intermolecular forces. The kinetic energy from temperature tends to push molecules apart. When temperature wins the competition, molecules fly apart and you have a gas. The intermolecular forces tend to bring molecules together. 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.

Strength of intermolecular forces

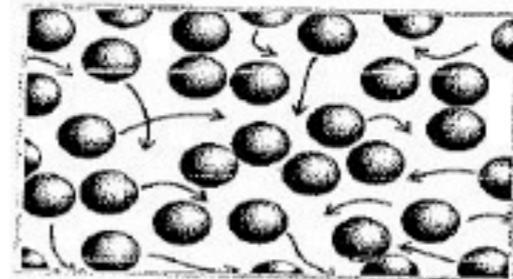
Iron is a solid at room temperature. Water is a liquid at room temperature. This tells you that the intermolecular forces between iron atoms are stronger than those between water molecules. In fact, iron is used for building things because it is so strong. The strength of solid iron is another effect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

Temperature

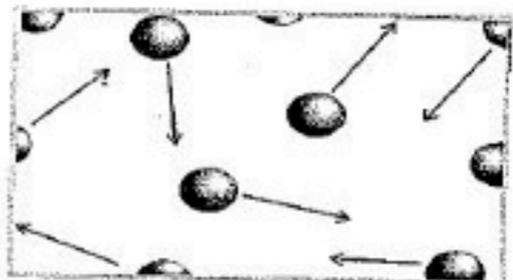
As the temperature changes, the balance between temperature and intermolecular forces changes. At temperatures below 0°C, the intermolecular forces in water are strong enough to overcome temperature and water becomes solid (ice).



Solid



Liquid



Gas

Figure 7.11: Molecules (or atoms) in the solid, liquid, and gas phases.

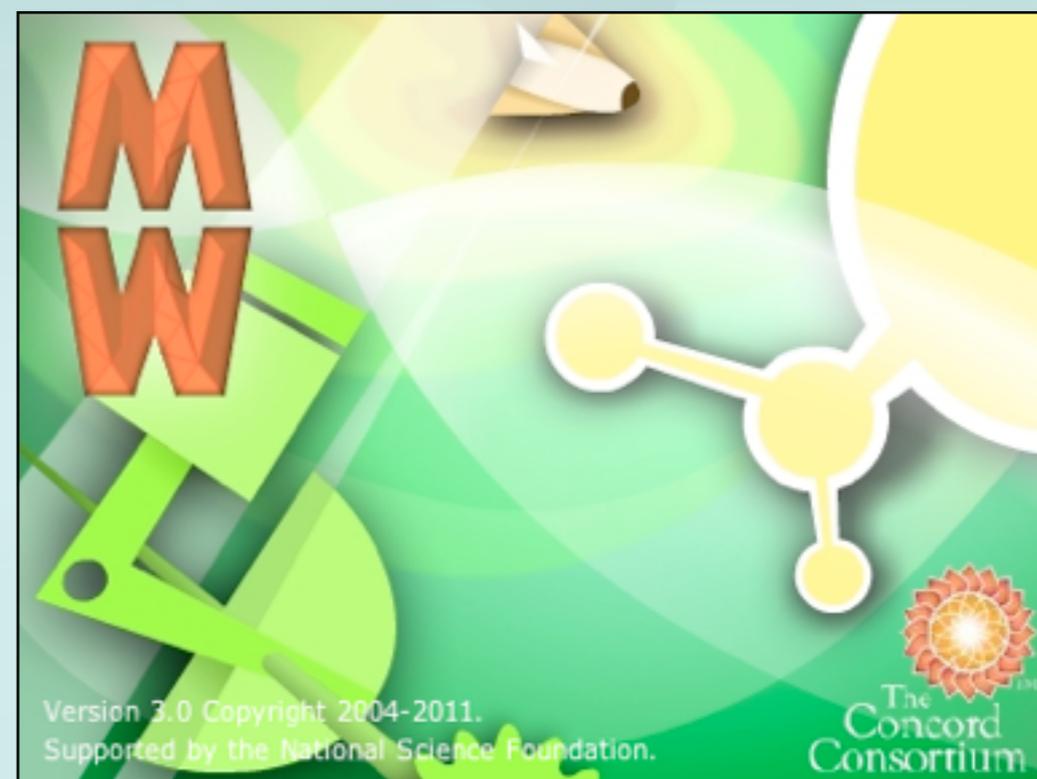
- Dynamic nature of atomic/molecular systems not easily conveyed with text and static images.
- Animations help, but don't allow students to construct knowledge. Student is passive learner.
- **Models which are computed in real-time allow users to probe the simulation by changing parameters. Student becomes an active learner.**

The Modeling Environment:

Molecular Workbench – a molecular dynamics tool.

The Molecular Workbench – a molecular dynamics tool.

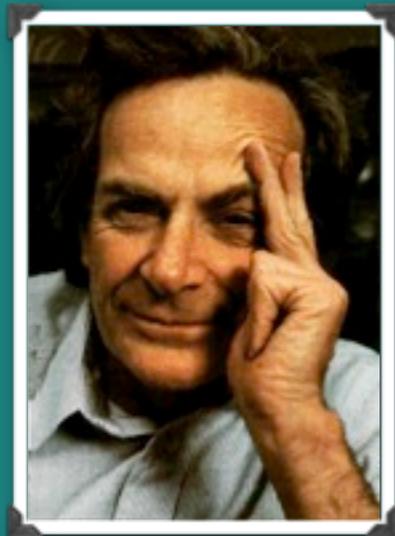
- Open-source cross-platform molecular dynamic engine.
- Calculates complex real-time interactions between atoms and molecules.
- User friendly interface for creating custom model-based activities.





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.

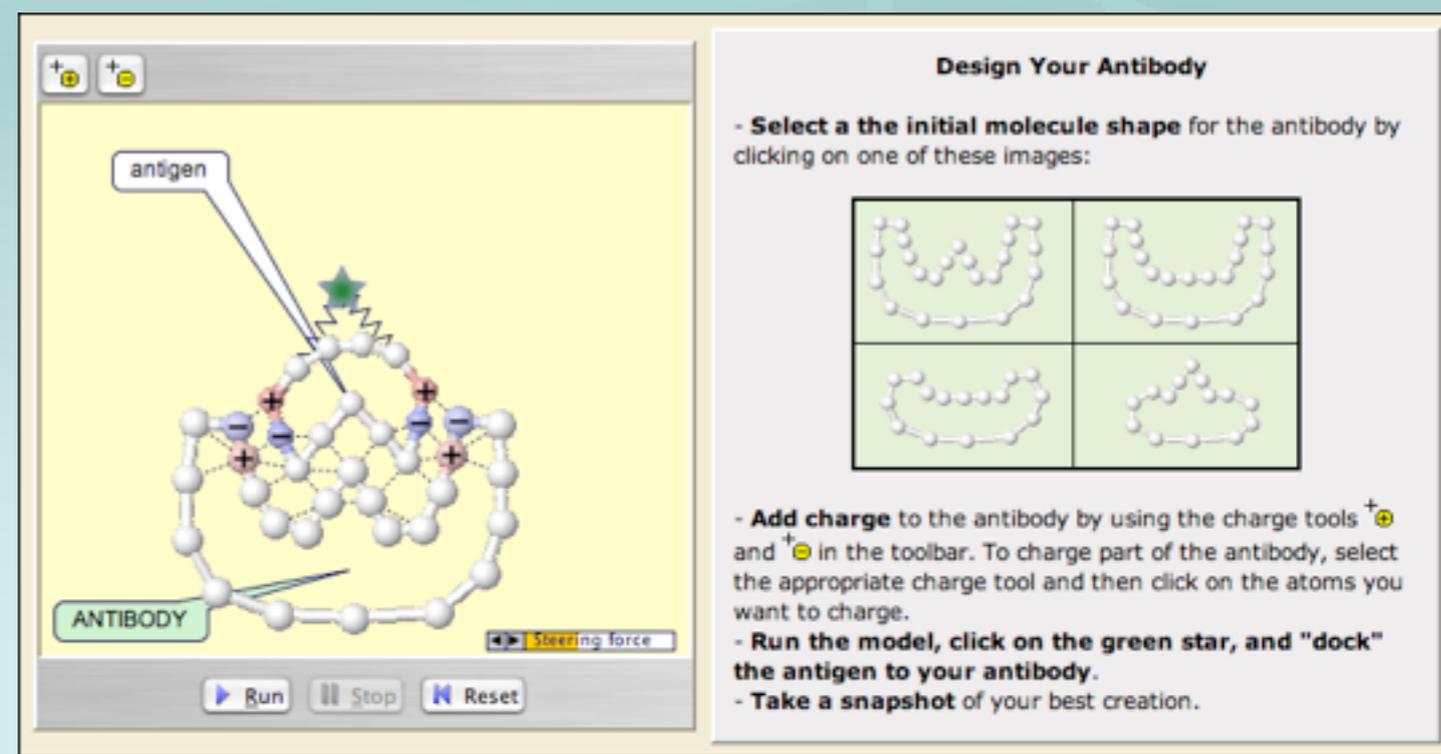
–Leon Lederman



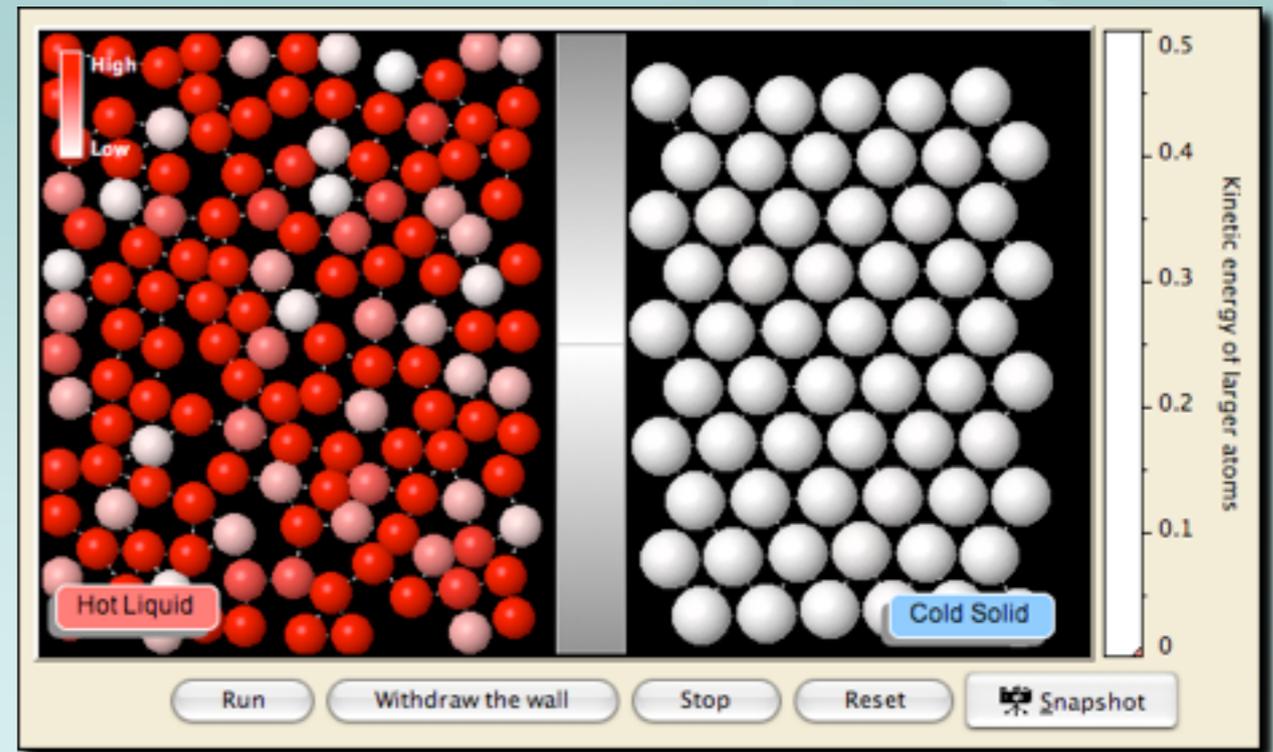
... all things are made of atoms — little particles that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another.

– Richard Feynman

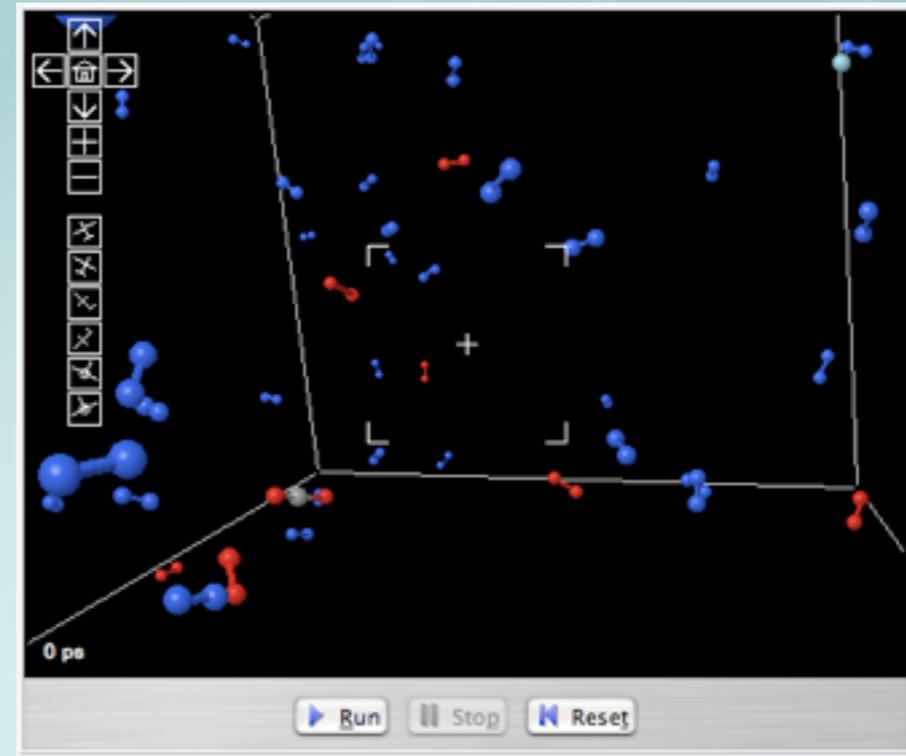
- 2D and 3D Molecular Dynamics Models
- 3D Exploration of Static Molecular Representation
- Flash based models
- Quantum physics - tunneling, bonding, time dependent Schrodinger representations
- Abstract dynamic models of DNA, RNA and proteins



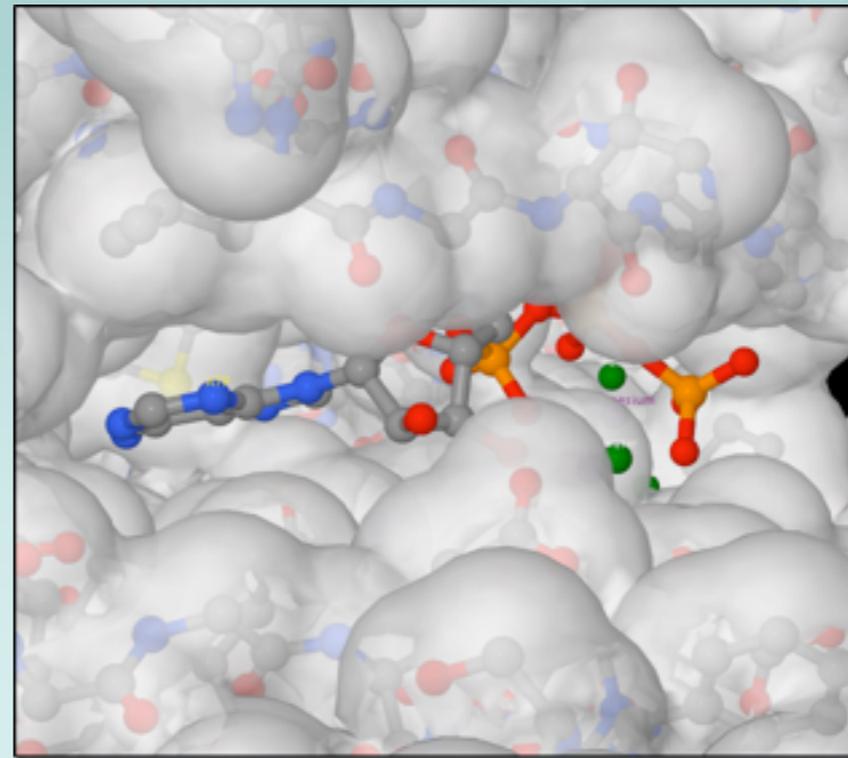
- 2D and 3D Molecular Dynamics Models
- 3D Exploration of Static Molecular Representation
- Flash based models
- Quantum physics - tunneling, bonding, time dependent Schrodinger representations
- Abstract dynamic models of DNA, RNA and proteins



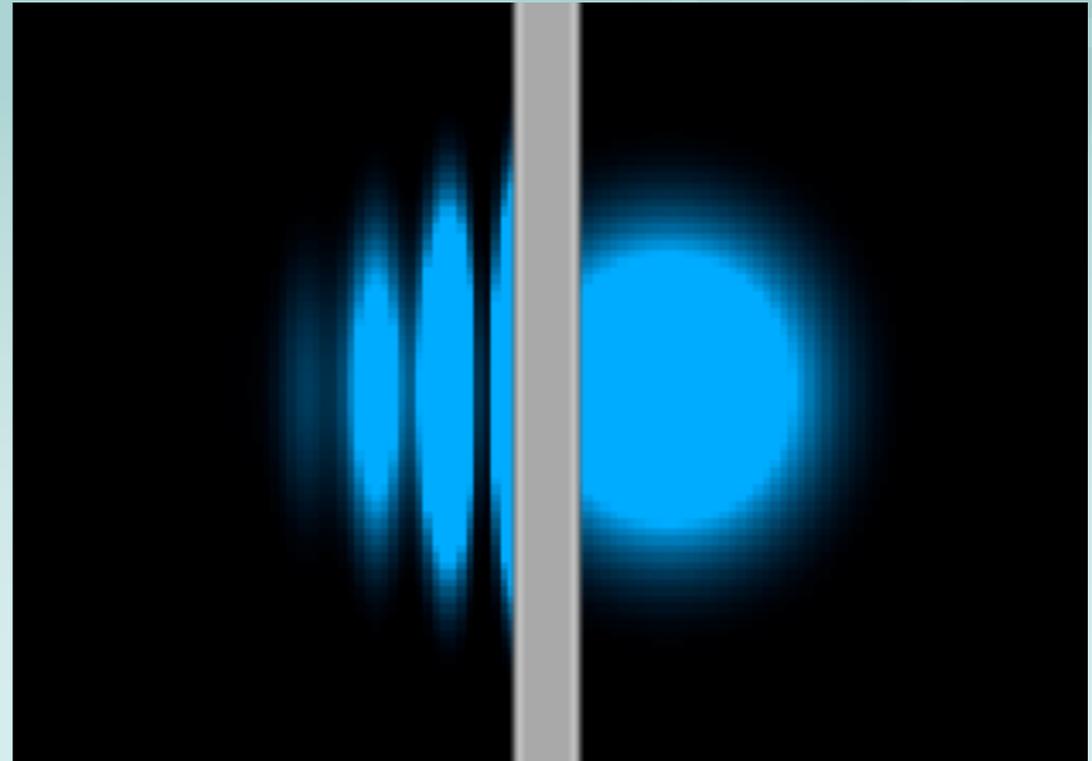
- 2D and 3D Molecular Dynamics Models
- 3D Exploration of Static Molecular Representation
- Flash based models
- Quantum physics - tunneling, bonding, time dependent Schrodinger representations
- Abstract dynamic models of DNA, RNA and proteins



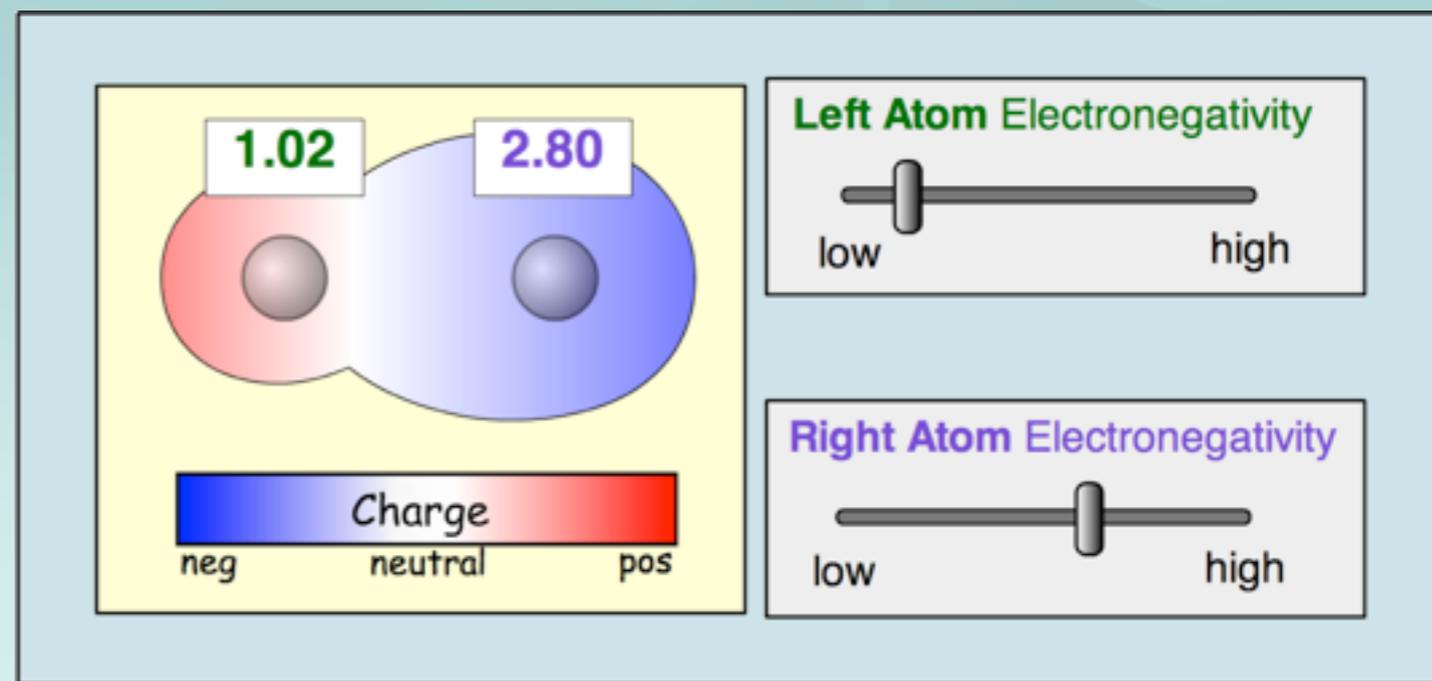
- 2D and 3D Molecular Dynamics Models
- 3D Exploration of Static Molecular Representation
- Flash based models
- Quantum physics - tunneling, bonding, time dependent Schrodinger representations
- Abstract dynamic models of DNA, RNA and proteins



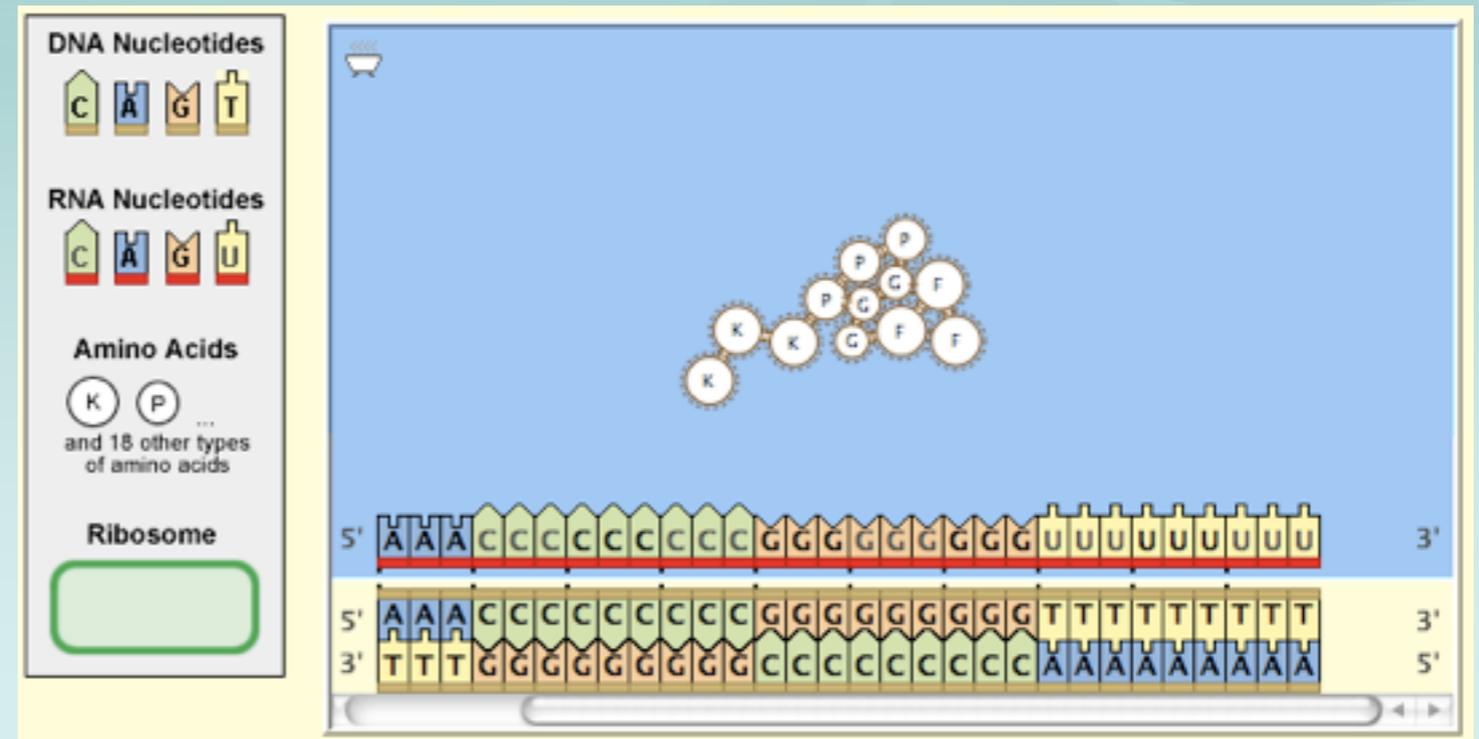
- 2D and 3D Molecular Dynamics Models
- 3D Exploration of Static Molecular Representation
- Flash based models
- Quantum physics - tunneling, bonding, time dependent Schrodinger representations
- Abstract dynamic models of DNA, RNA and proteins



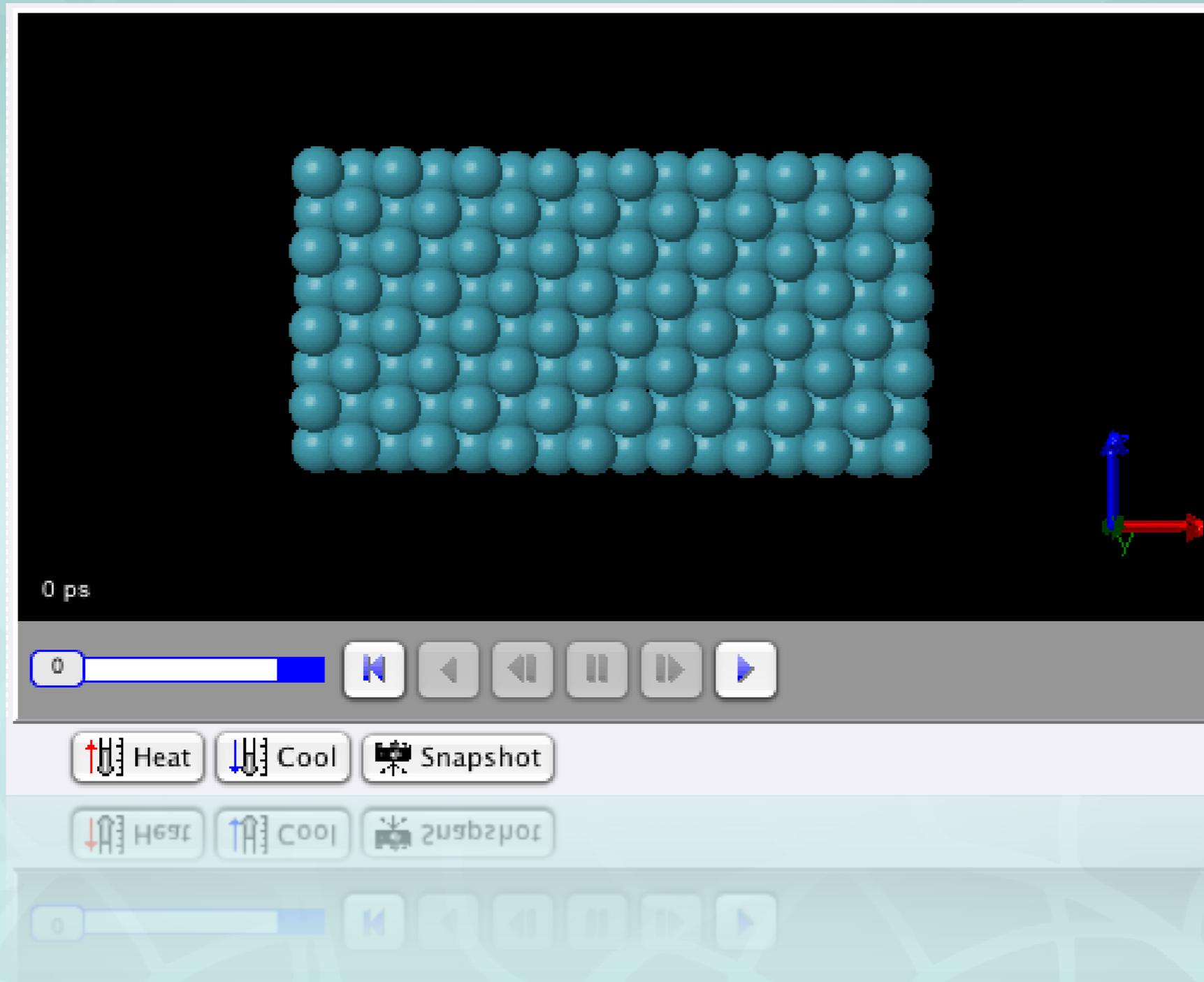
- 2D and 3D Molecular Dynamics Models
- 3D Exploration of Static Molecular Representation
- Flash based models
- Quantum physics - tunneling, bonding, time dependent Schrodinger representations
- Abstract dynamic models of DNA, RNA and proteins



- 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



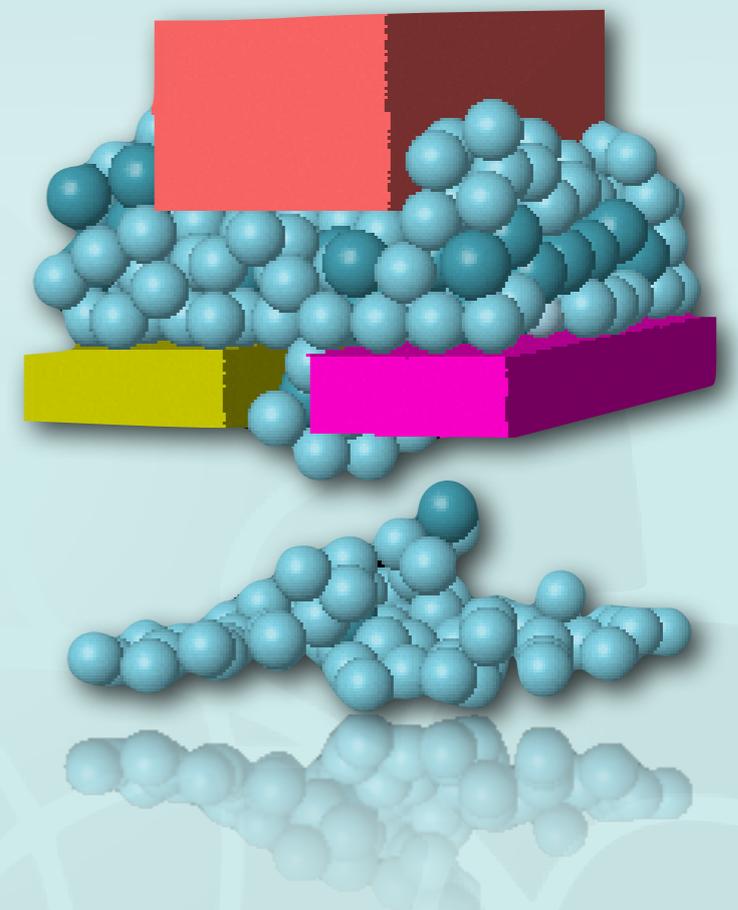
Dynamic Phase Change Model



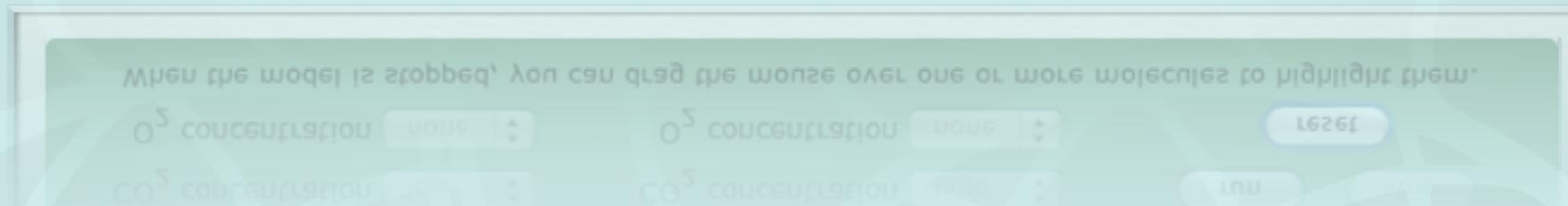
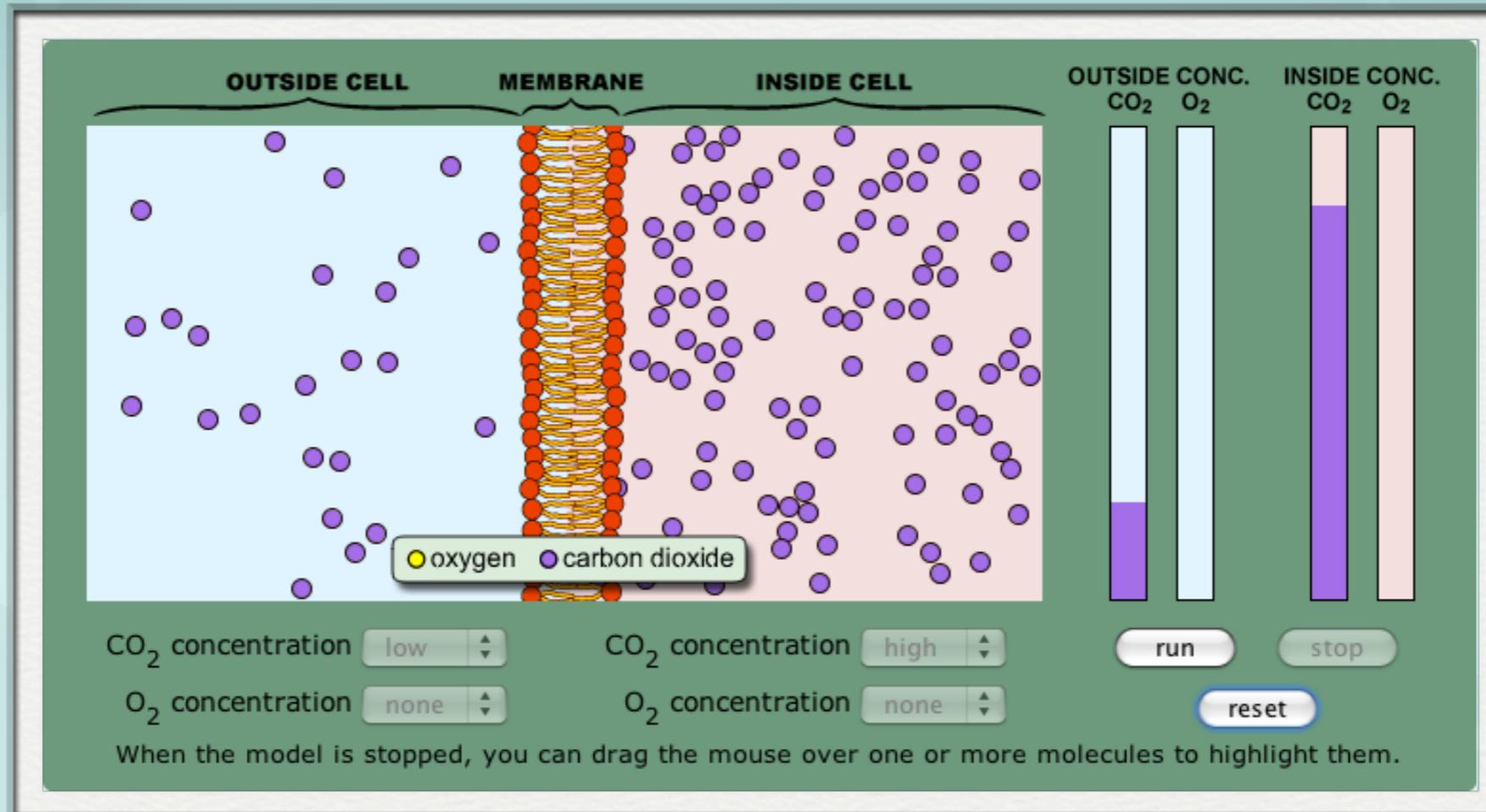
The screenshot displays a simulation window with a black background. In the center, a rectangular lattice of blue spheres is shown, representing a solid phase. To the right of the lattice, a 3D coordinate system is visible with three axes: a vertical blue axis pointing upwards, a horizontal red axis pointing to the right, and a diagonal green axis pointing downwards and to the right. Below the simulation area, the text "0 ps" is displayed. A control panel is located at the bottom of the window, featuring a progress bar with a blue slider and a "0" label, followed by navigation buttons: a blue play button, a grey left arrow, a grey double left arrow, a grey pause button, a grey double right arrow, and a blue right arrow. Below these buttons are three control buttons: "Heat" (with a red up arrow and a blue down arrow), "Cool" (with a blue down arrow and a red up arrow), and "Snapshot" (with a camera icon). A second, semi-transparent control panel is visible below the first one, containing mirrored buttons for "Heat", "Cool", and "Snapshot".

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.



Biology - Equilibrium



Biology - DNA to Proteins

Key

DNA Nucleotides

C A G T

RNA Nucleotides

C A G U

Amino Acids

● Hydrophilic

● Hydrophobic

5' **A G A T T T G G G C T C A T G C T A G C T A T A G T A C T T T A G** 3'

3' **T C T A A A C C C G A G T A C G A T C G A T A T C A T G A A A T C** 5'



Transcribe DNA to mRNA

Translate mRNA to protein

Take a snapshot

[Genetic Code Table](#)

Transcribe DNA to mRNA

Translate mRNA to protein

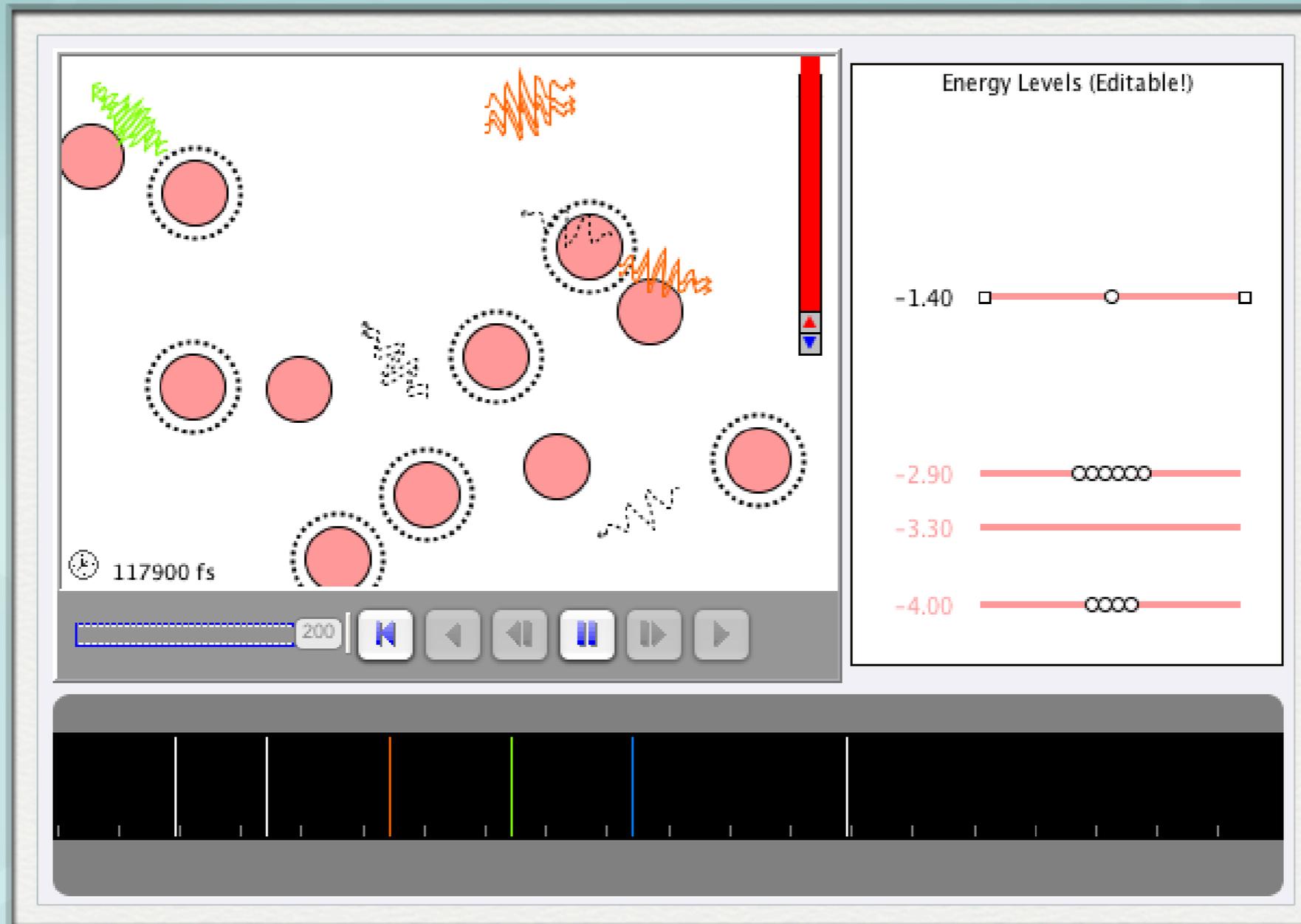
Take a snapshot



3' T C T A A A C C C G A G T A C G A T C G A T A T C A T G A A A T C 5'

[Genetic Code Table](#)

Phys/Chem - Spectroscopy



Follow these steps:

1. Add some atoms (press multiple times to add more):

add 2

add 10

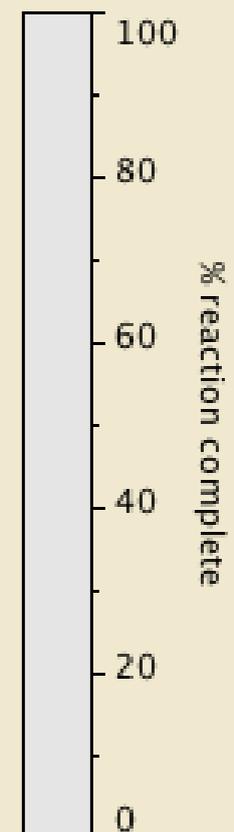
2. Run ▶ the model.

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.



Your Goal: $\bullet + \bullet \rightarrow \bullet\text{---}\bullet$
To get atoms to react to form molecules.

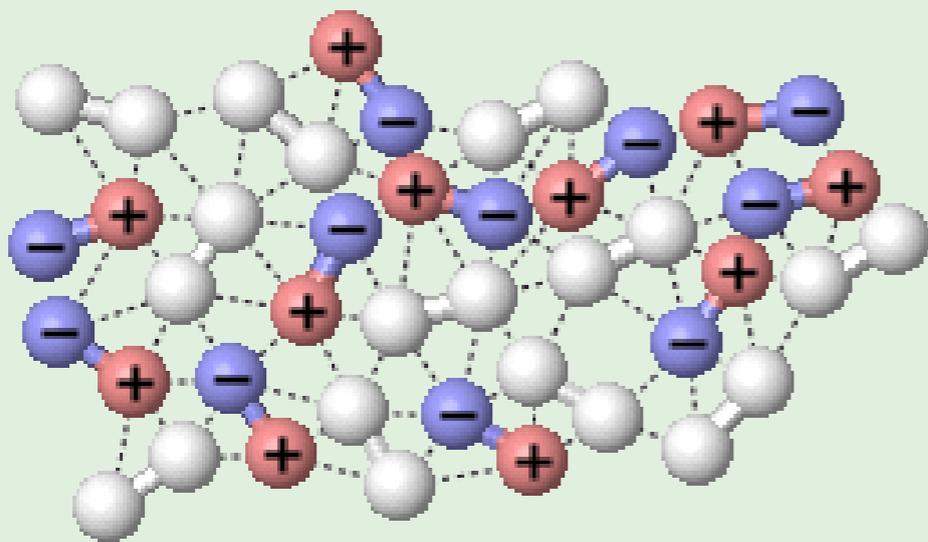


reaches 80% completion:
the graph to see when the reaction
reaches 80% completion.



Chem/Bio - Intermolecular Attractions

Oil and Water Shaken Up and Mixed



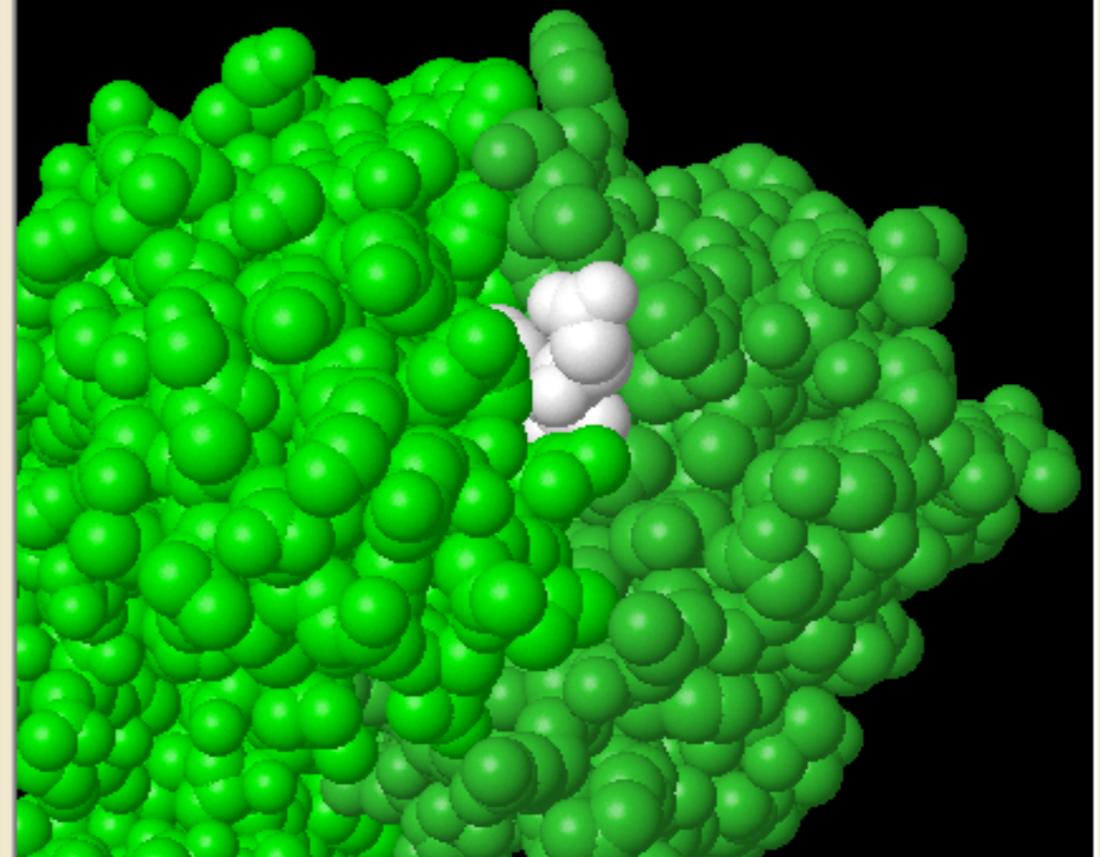
press run to see the mixture "settle"

▶ Run

⏸ Stop

⏪ Reset

Antibody/Antigen



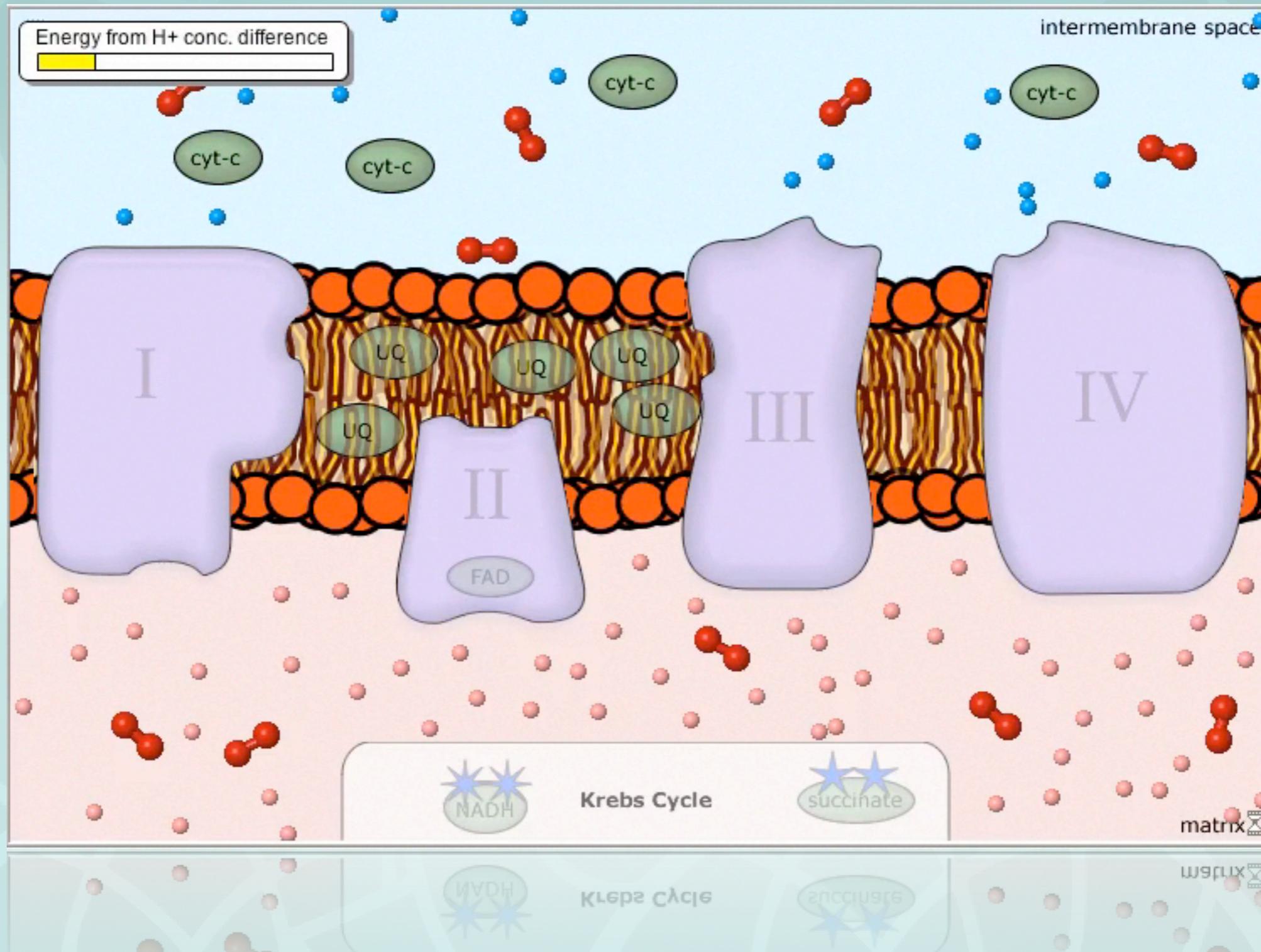
▶ Run

⏸ Stop

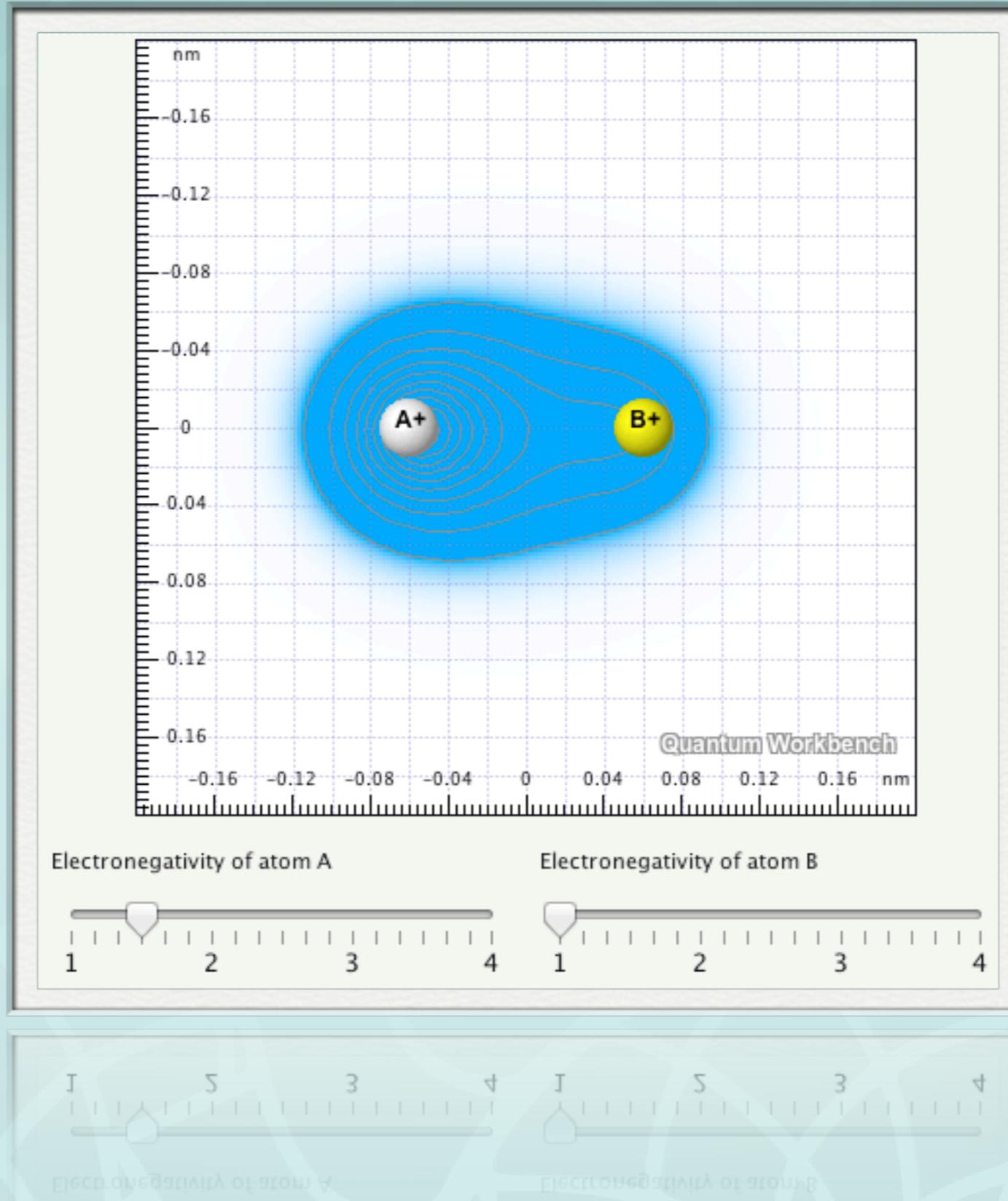
⏪ Reset

press run to see the mixture "settle"

Modeling Macro-level Systems the electron transport chain



Quantum Chemistry - Polar Bonds



Embedded Assessments

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.

Check Answer

Embedded Assessments

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

Embedded Assessments

Describe how the chemical energy in ATP is converted into electric potential energy. ([hint](#))

Embedded Assessments

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.

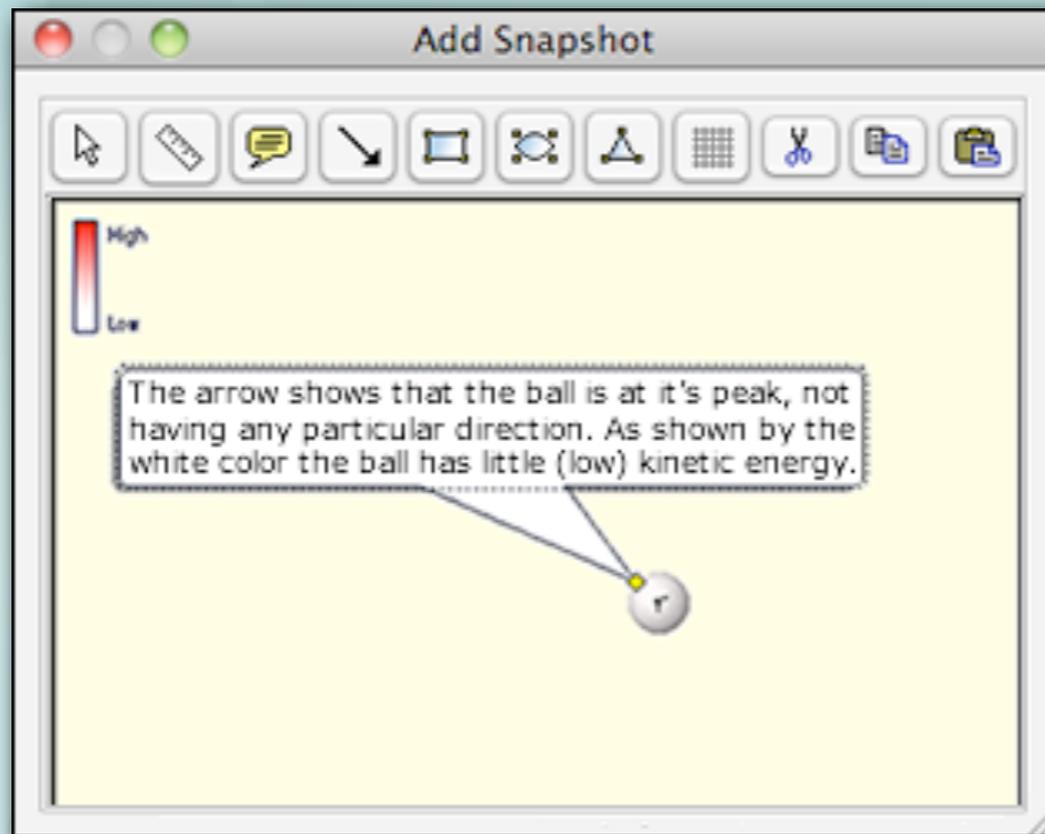
Click the Open Button,
and then drag a thumbnail here.

Open

Clear

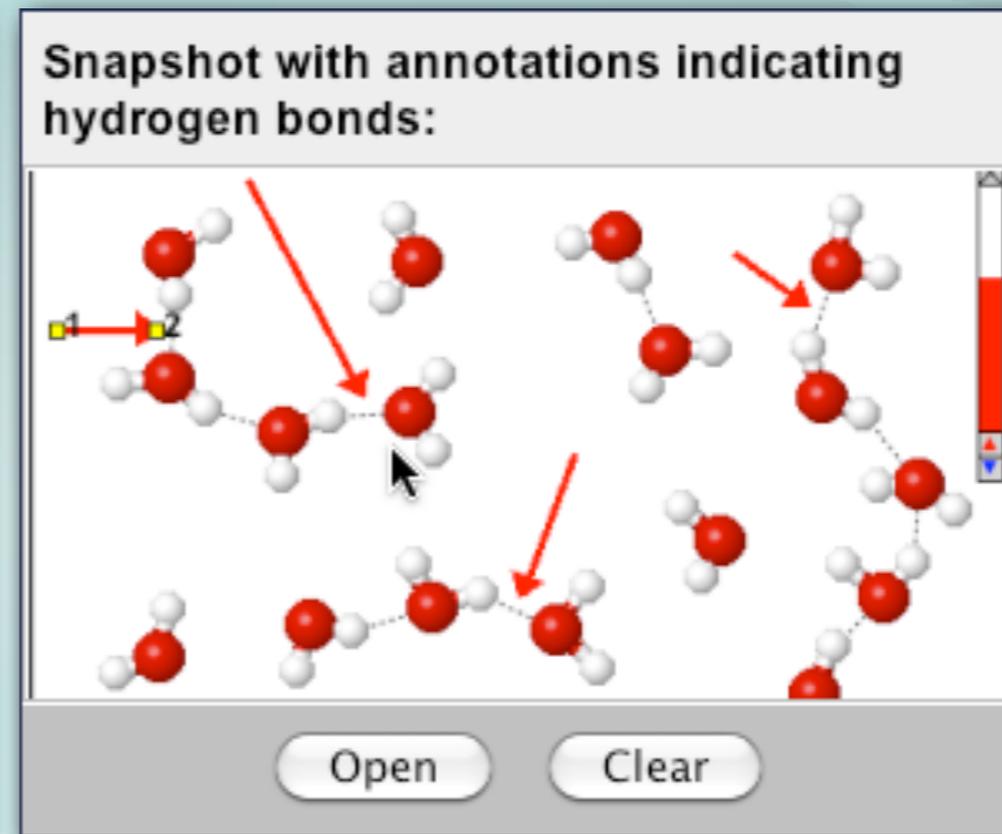
Embedded Assessments

Add Snapshot



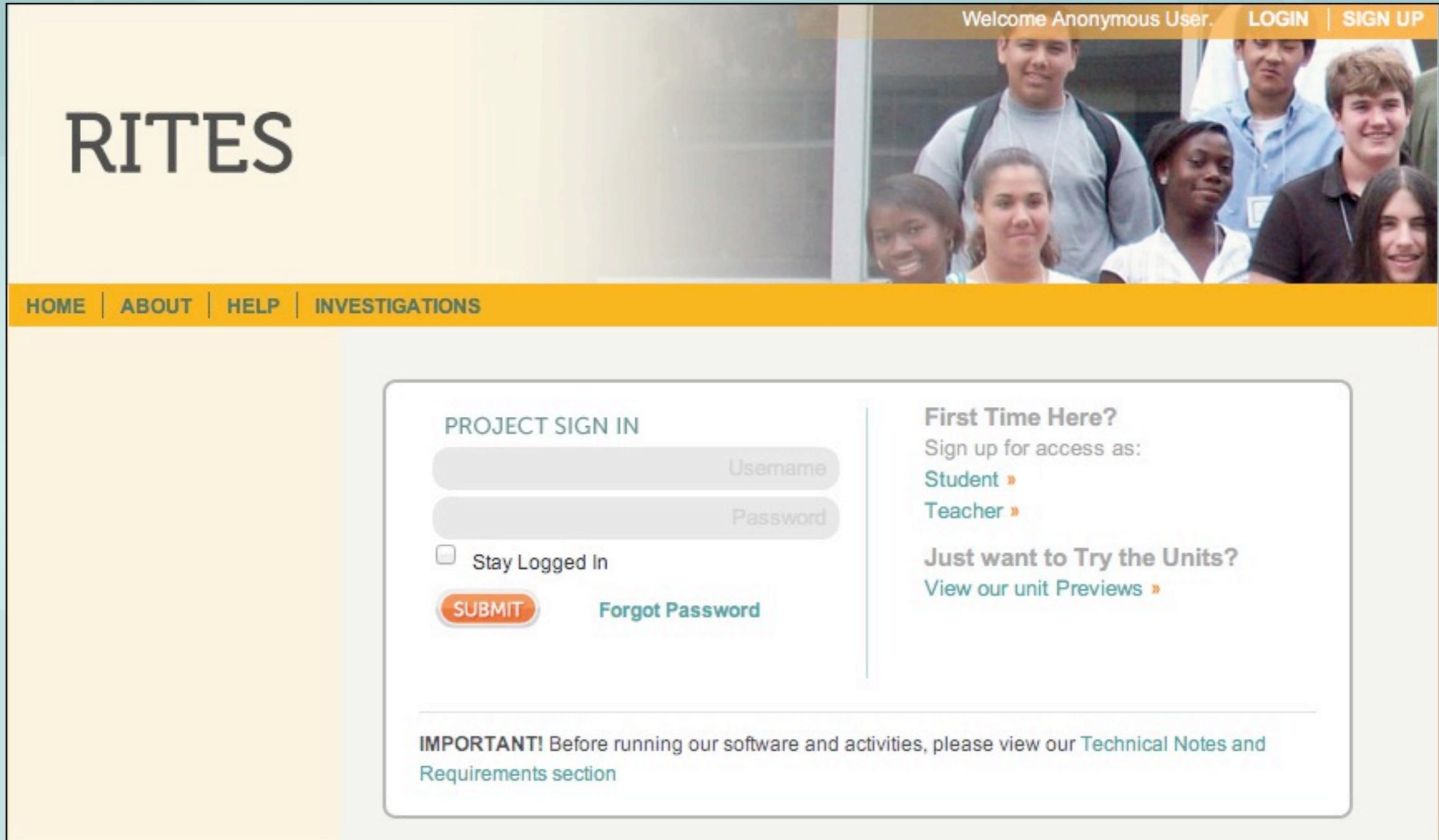
The arrow shows that the ball is at it's peak, not having any particular direction. As shown by the white color the ball has little (low) kinetic energy.

Snapshot with annotations indicating hydrogen bonds:



Open Clear

Previewing Models and Using a Portal



The screenshot shows the RITES portal homepage. At the top right, it says "Welcome Anonymous User." with links for "LOGIN" and "SIGN UP". The main header features the word "RITES" in large letters. Below this is a navigation bar with links for "HOME", "ABOUT", "HELP", and "INVESTIGATIONS". The central content area is divided into two columns. The left column is titled "PROJECT SIGN IN" and contains input fields for "Username" and "Password", a "Stay Logged In" checkbox, a "SUBMIT" button, and a "Forgot Password" link. The right column is titled "First Time Here?" and offers options to sign up as a "Student" or "Teacher". Below this, it asks "Just want to Try the Units?" and provides a link to "View our unit Previews". At the bottom of the page, an "IMPORTANT!" notice advises users to view "Technical Notes and Requirements section" before using the software.

Welcome Anonymous User. [LOGIN](#) | [SIGN UP](#)

RITES

[HOME](#) | [ABOUT](#) | [HELP](#) | [INVESTIGATIONS](#)

PROJECT SIGN IN

Username

Password

Stay Logged In

[SUBMIT](#) [Forgot Password](#)

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](#)

Student Quotes

“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.”

Student Quotes

“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.”

Teacher Quotes of Their “Best Experiences”

“In a lesson on electrostatics (not the RI-ITEST model) a student referred back to something he had learned while doing a RI-ITEST activity. The classroom discussion went far more smoothly as a result of the students having learned about atomic structure via the interactive models.

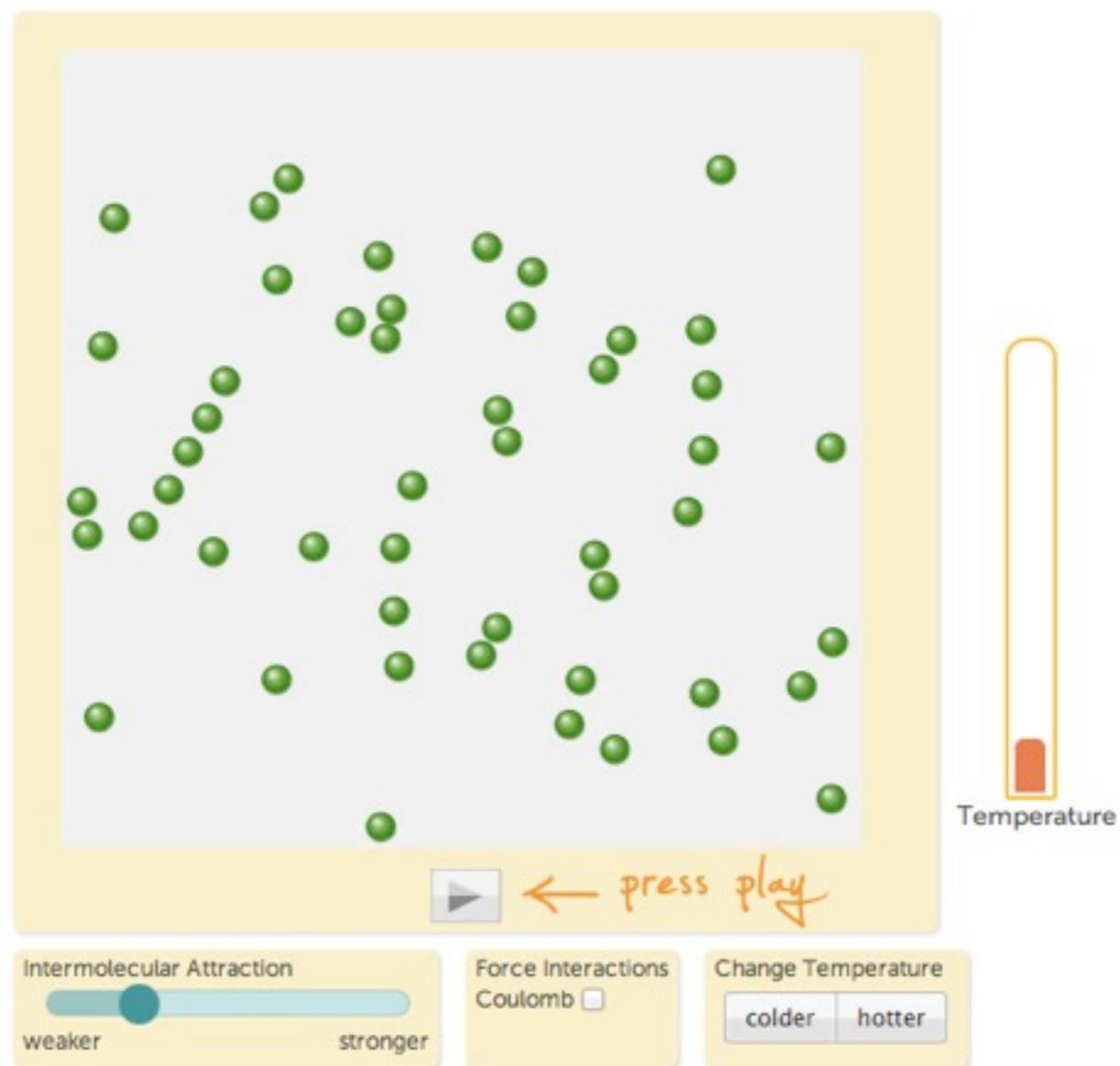
Teacher Quotes of Their “Best Experiences”

“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.



The screenshot shows a simulation window with a light gray background and a yellow border. Inside, numerous green spheres representing atoms are scattered. To the right of the window is a vertical thermometer with a red liquid level and the label "Temperature". Below the window is a play button icon with a handwritten orange arrow pointing to it and the text "press play". At the bottom, there are three control panels: "Intermolecular Attraction" with a slider from "weaker" to "stronger"; "Force Interactions" with a checkbox for "Coulomb"; and "Change Temperature" with "colder" and "hotter" buttons.

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.

- Science of Atoms and Molecules (SAM/RI-ITEST)

- High Adventure Science

- Geniverse

- Evolution Readiness

- Electron Technologies

- Innovative Technology in Science Inquiry (ITSI-SU)

- Engineering Energy Efficiency



Science of Atoms and Molecules

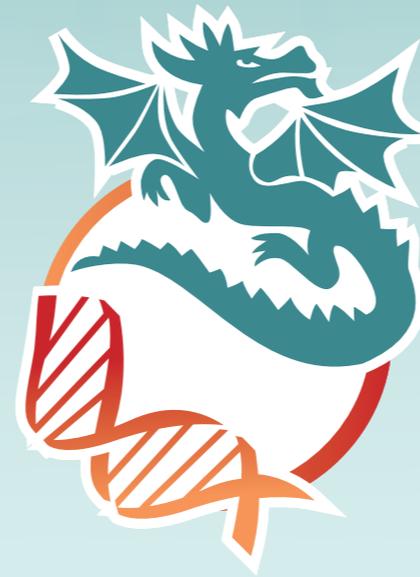
- Science of Atoms and Molecules (SAM/RI-ITEST)
- High Adventure Science
- Geniverse
- Evolution Readiness
- Electron Technologies
- Innovative Technology in Science Inquiry (ITSI-SU)
- Engineering Energy Efficiency



High-Adventure Science

Finding Models and Activities - Current and Past Projects

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



Geniverse

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



Evolution Readiness



Finding Models and Activities - Current and Past Projects

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



Electron Technologies

Finding Models and Activities - Current and Past Projects

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



ITSI-SU

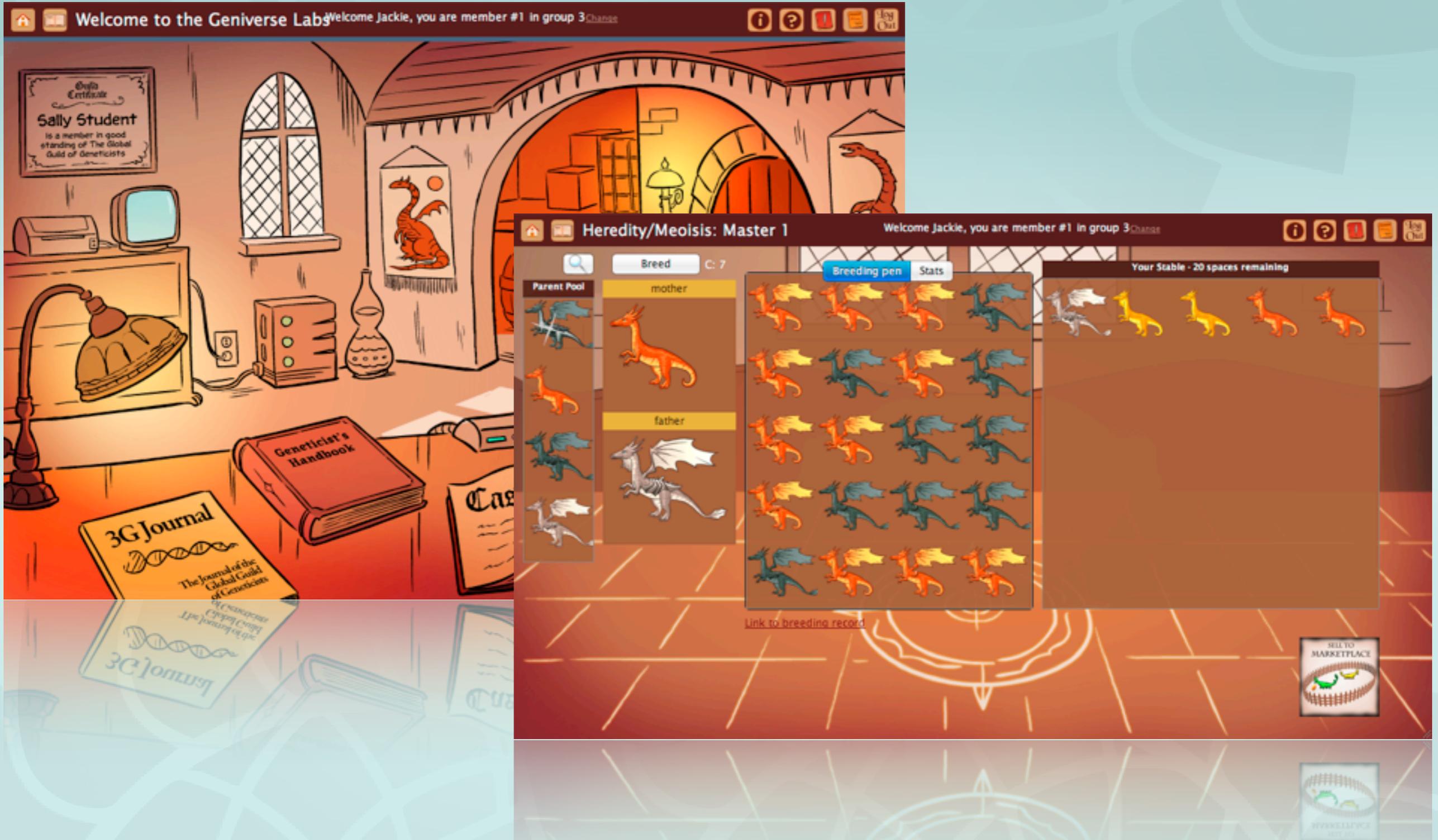
Finding Models and Activities - Current and Past Projects

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



**Engineering
Energy Efficiency**

Geniverse



The screenshot displays the Geniverse Lab interface, which is divided into two main sections: a virtual laboratory and a breeding simulation.

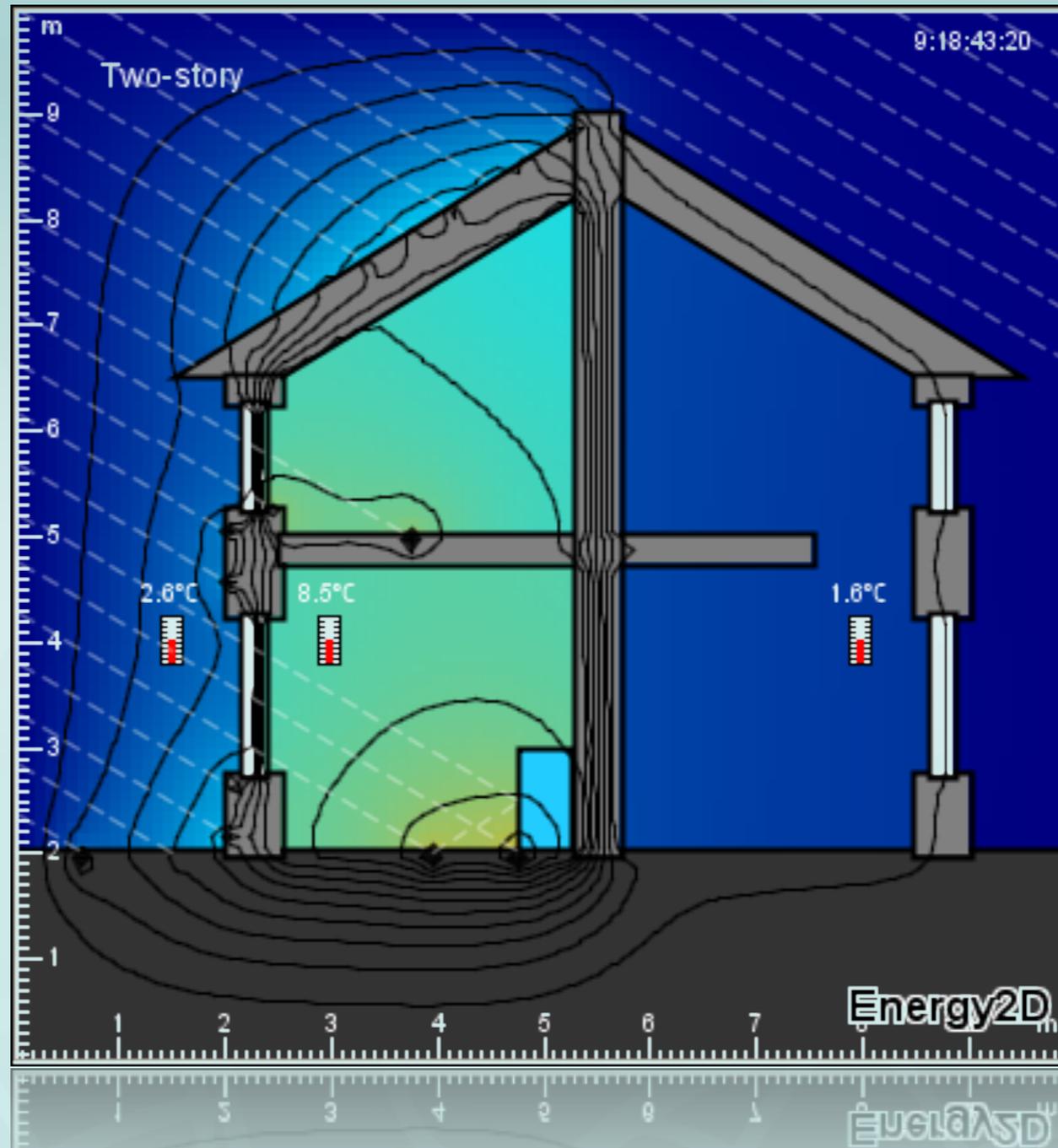
Virtual Laboratory (Left): The scene is a cartoon-style laboratory. On the left, a desk holds a computer monitor, a printer, and a lamp. A framed certificate on the wall reads "Diploma Certificate Sally Student is a member in good standing of The Global Guild of Geneticists". In the center, a window looks out onto a building with a dragon-shaped poster. On the right, a doorway leads to a stable area where a dragon is visible. On the desk in the foreground, there is a "3G Journal" (The Journal of the Global Guild of Geneticists), a "Geneticist's Handbook", and a "Case" file.

Breeding Simulation (Right): The interface is titled "Heredity/Meiosis: Master 1". It features a "Breed" button and a "C: 7" indicator. The simulation is organized into several panels:

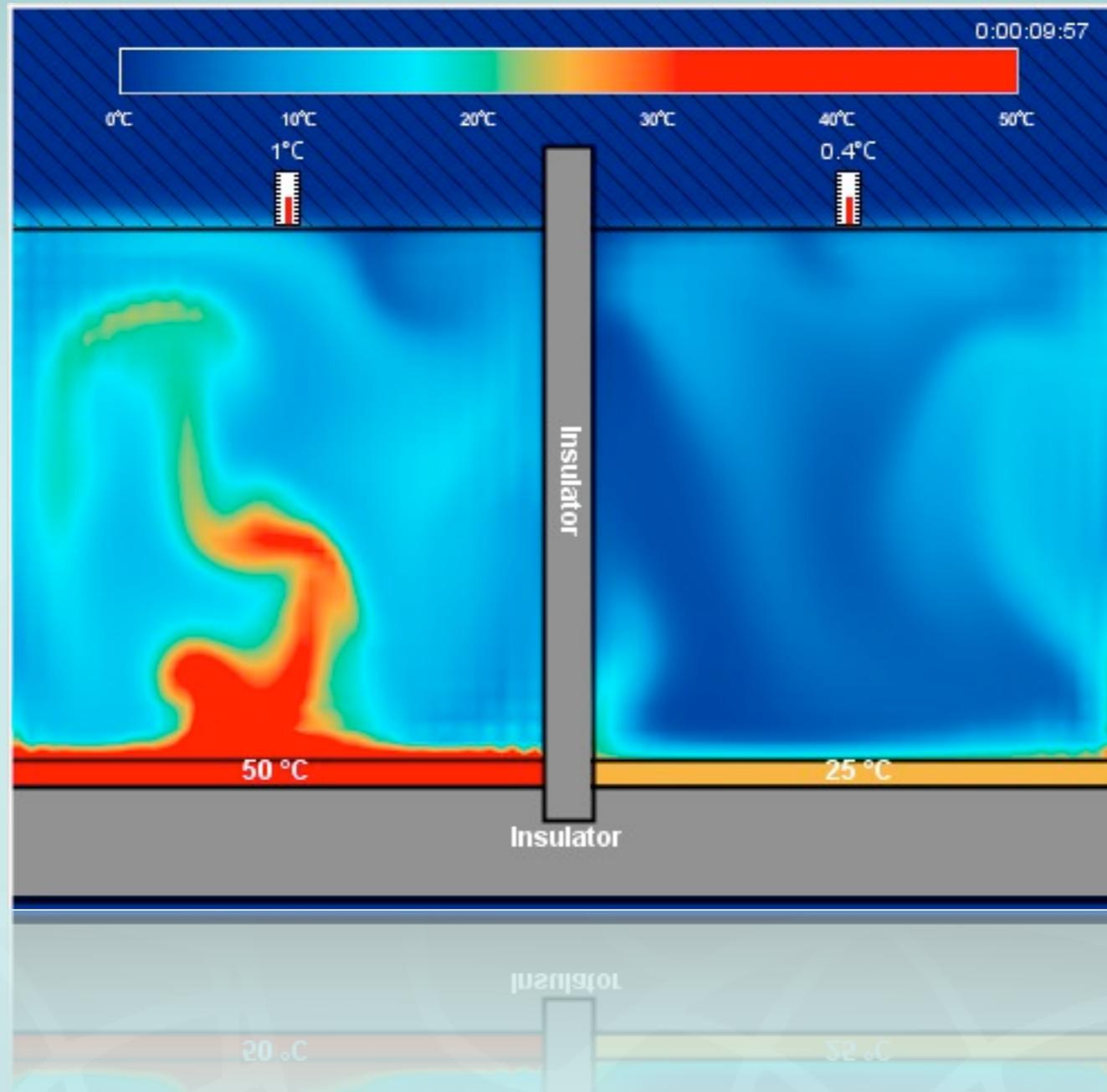
- Parent Pool:** A vertical list of dragon icons representing the genetic pool.
- mother:** A panel showing the selected mother dragon, an orange dragon.
- father:** A panel showing the selected father dragon, a white dragon.
- Breeding pen:** A grid of 20 dragon icons representing the offspring of the current pair.
- Stats:** A panel with a "Link to breeding record" button.
- Your Stable - 20 spaces remaining:** A horizontal row of 20 dragon icons representing the current stable population.

At the bottom right of the interface, there is a "SELL TO MARKETPLACE" button with a circular icon containing a dragon.

Design Principles



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

Dan Damelin

dan@concord.org

<http://www.concord.org>

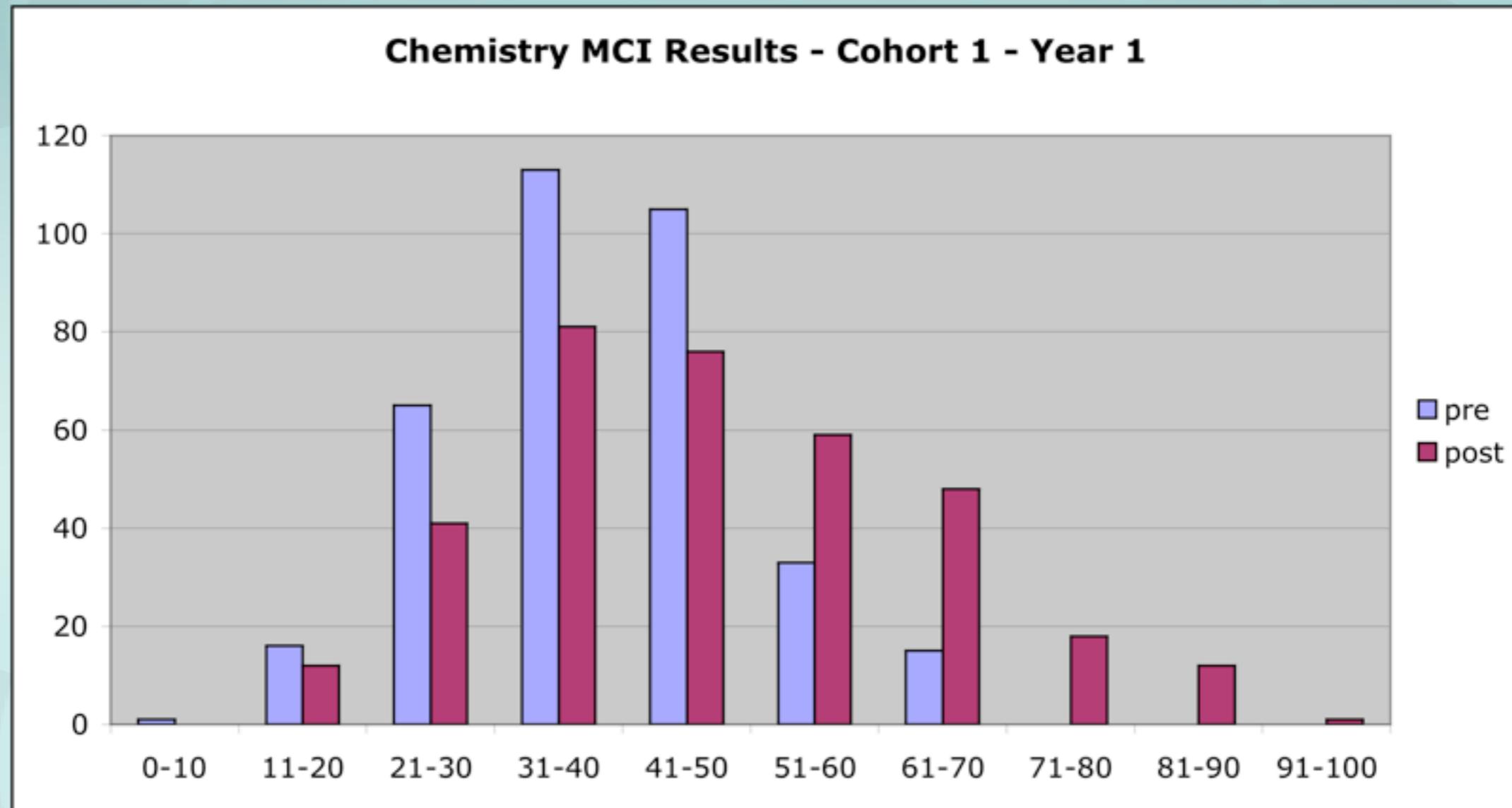
subscribe to our newsletter

RI-ITEST Project

	PHYSICS	CHEMISTRY	BIOLOGY
MOTION AND ENERGY	Atoms and Energy	Phase Change	Diffusion, Osmosis, and Active Transport
	Heat and Temperature	Gas Laws	Cellular Respiration
CHARGE	Electrostatics	Intermolecular Attractions	Four Levels of Protein Structure
	Electricity	Molecular Geometry	Protein Partnering and Function
		Solubility	
ATOMS AND MOLECULES	Atomic Structure	Chemical Bonds	Intro to Macromolecules
	Newton's Laws at the Atomic Scale	Chemical Reactions and Stoichiometry	Lipids and Carbohydrates
			Nucleic Acids and Proteins
			DNA to Proteins
LIGHT	Atoms, Excited States, and Photons		Harvesting Light for Photosynthesis
	Spectroscopy		

MCI Results

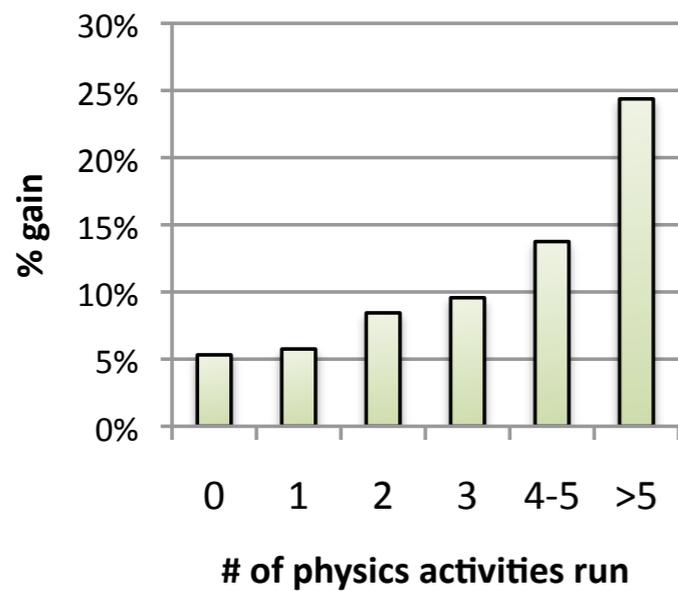
Cohort 1 - Chem



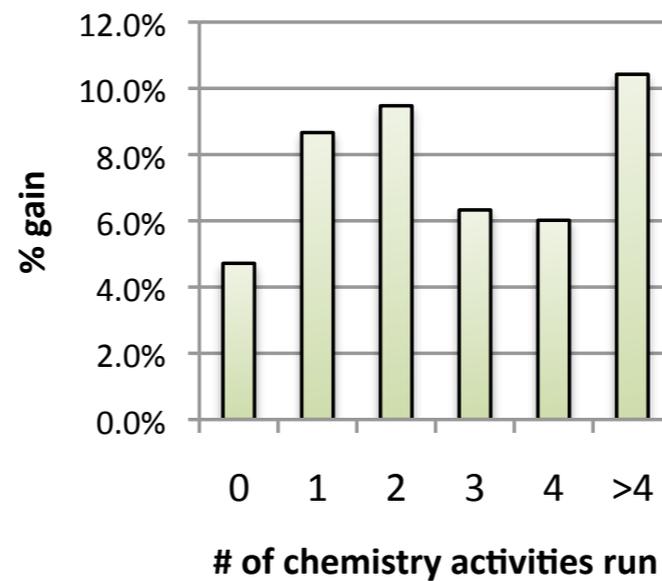
Group	Pre-test mean	Post-test mean	n	p-value based on paired t-test	Cohen's d	Effect size
Chemistry	39%	47%	348	7.8e-32	0.6	Moderate

Score increases related to number of SAM activities completed

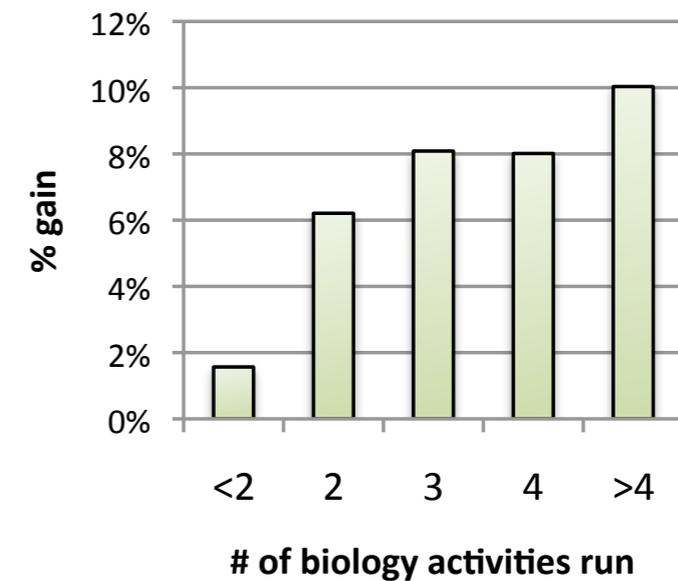
MCI gain vs. # of physics activities run
(cohort 2 - year 2)



MCI gain vs. # of chemistry activities run
(cohort 2 - year 2)



MCI gain vs. # of bio activities run
(cohort 2 - year 2)



Improvements Over Time

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