



The Concord
Consortium

Using the Molecular Workbench for Inquiry at the Atomic Level

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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.

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

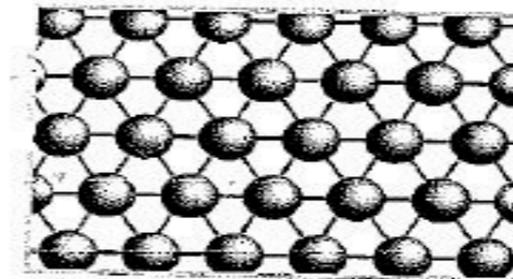
Within all matter there is a constant competition between temperature and intermolecular forces. The kinetic energy from temperature tends to push molecules apart. When temperature wins the competition, molecules fly apart and you have a gas. The intermolecular forces tend to bring molecules together.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

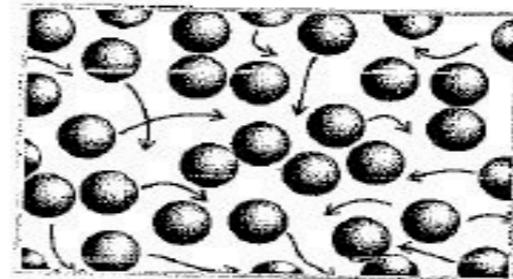
Iron is a solid at room temperature. Water is a liquid at room temperature. This tells you that the intermolecular forces between iron atoms are stronger than those between water molecules. In fact, iron is used for building things because it is so strong. The strength of solid iron is another effect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

Temperature

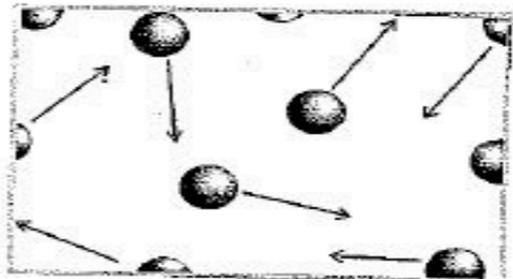
As the temperature changes, the balance between temperature and intermolecular forces changes. At temperatures below 0°C, the intermolecular forces in water are strong enough to overcome temperature and water becomes solid (ice).



Solid



Liquid



Gas

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

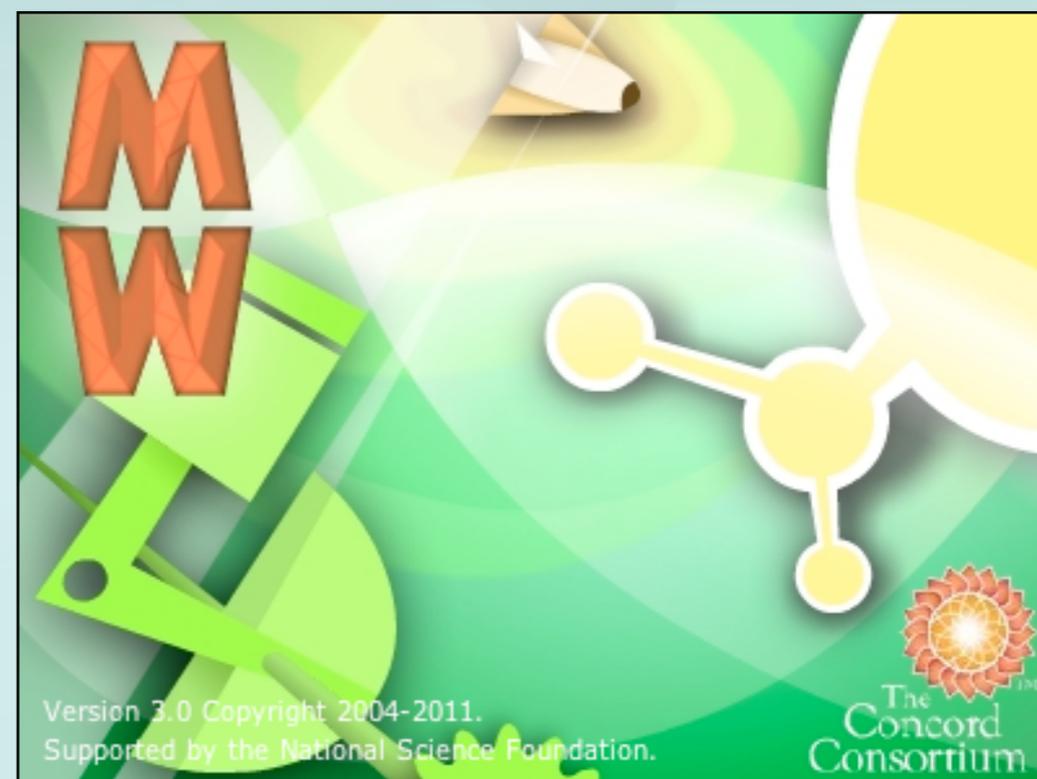
- Dynamic nature of atomic/molecular systems not easily conveyed with text and static images.
- Animations help, but don't allow students to construct knowledge. Student is passive learner.
- **Models which are computed in real-time allow users to probe the simulation by changing parameters. Student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

The Modeling Environment:

Molecular Workbench – a molecular dynamics tool.

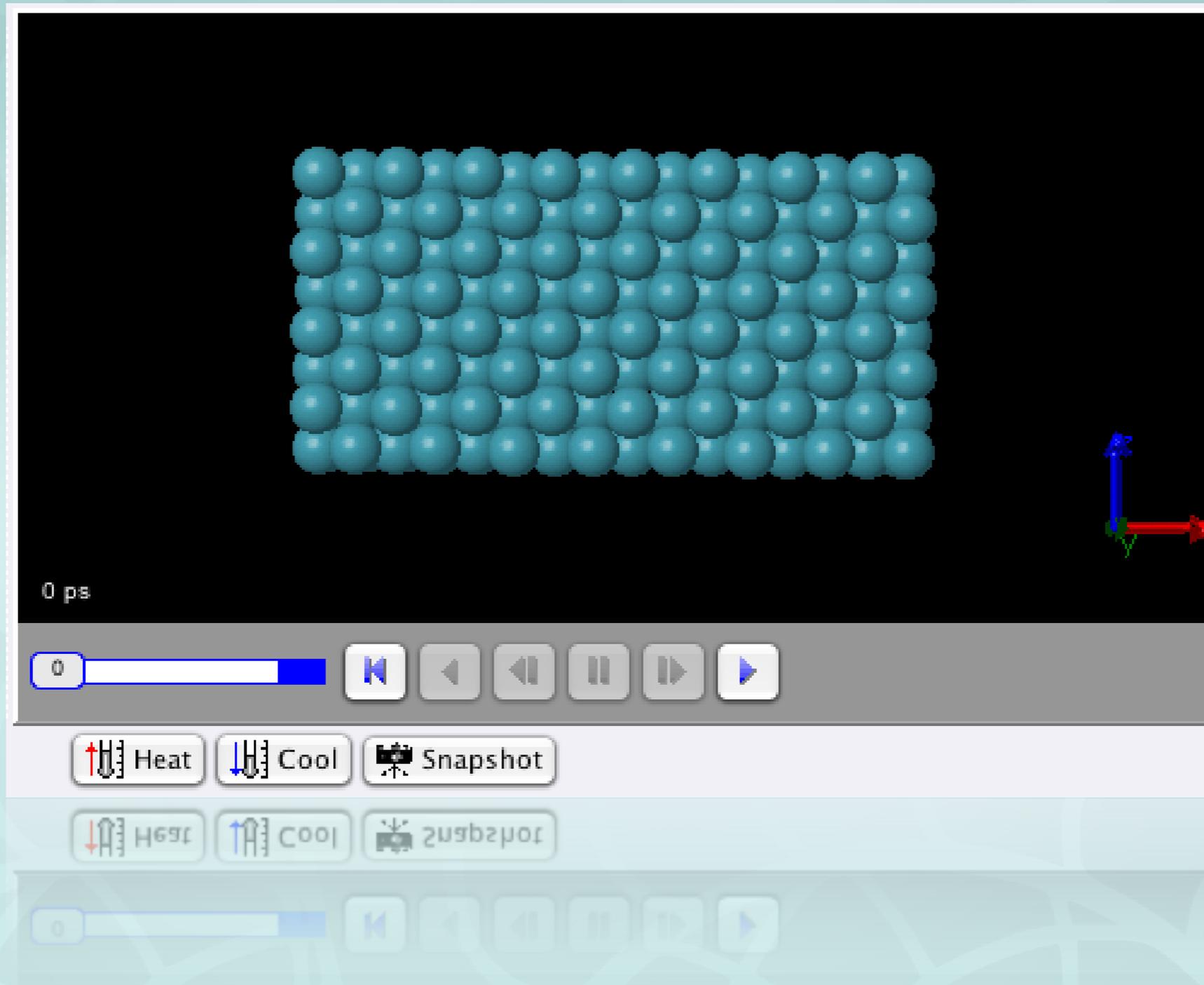
The Molecular Workbench – a molecular dynamics tool.

- 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.



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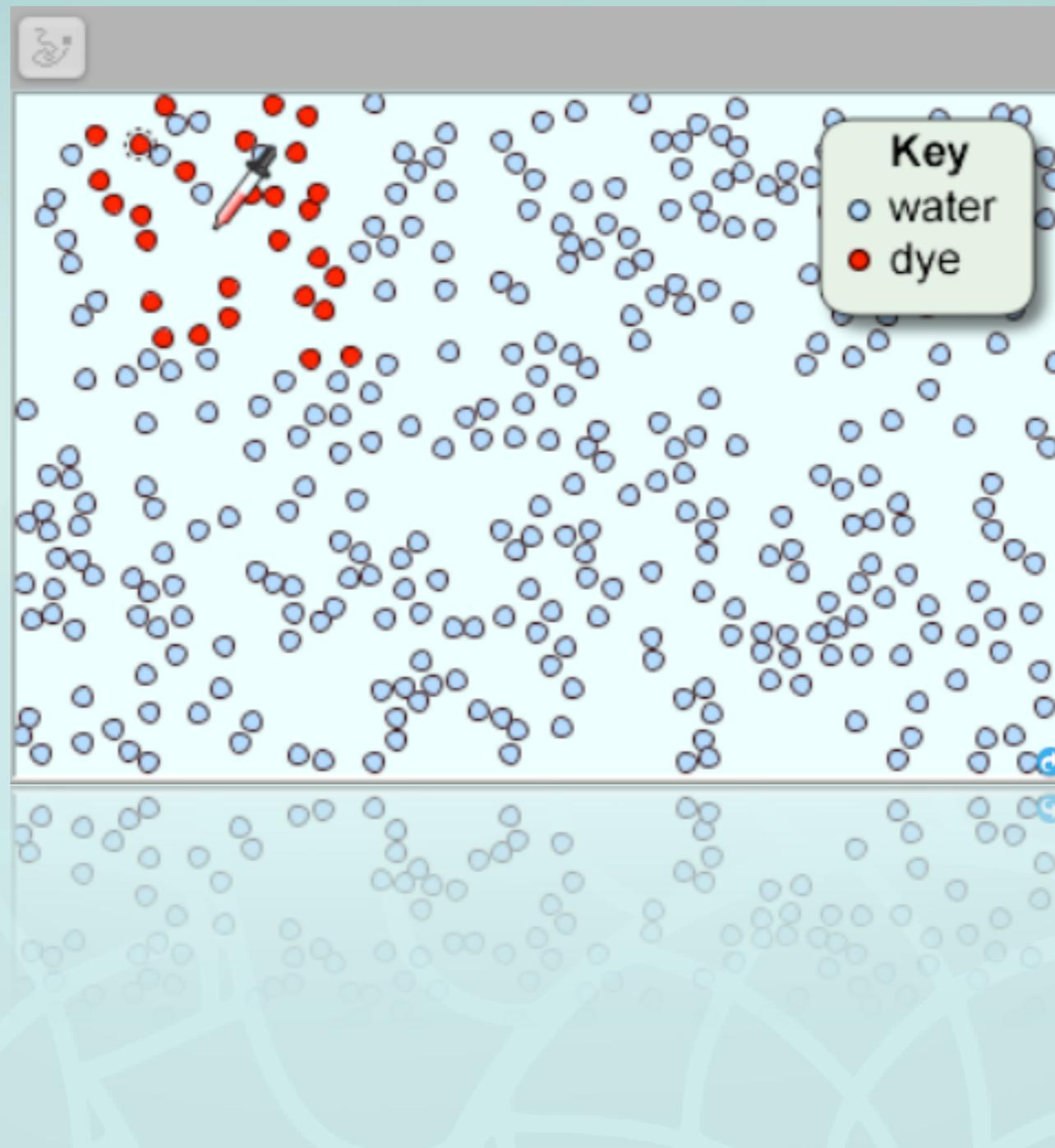
Dynamic Phase Change Model



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 buttons labeled "Heat", "Cool", and "Snapshot". The "Heat" button has a red upward arrow, "Cool" has a blue downward arrow, and "Snapshot" has a camera icon. A second, semi-transparent control panel is visible below the first one, with the labels "Heat", "Cool", and "Snapshot" mirrored and inverted.

2D Dynamic Motion

simple diffusion



Follow these steps:

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

add 2

add 10

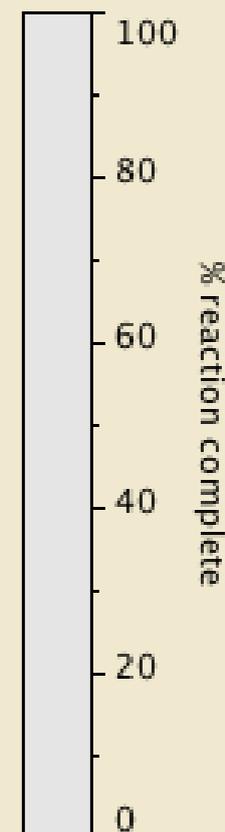
2. Run ▶ the model.

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.

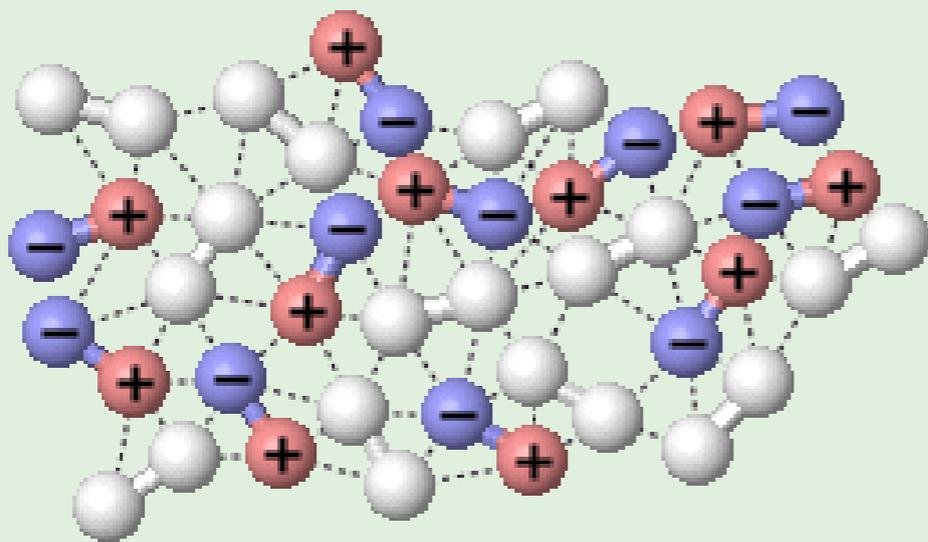


reaches 80% completion:
the graph to see when the reaction
reaches 80% completion.



Chem/Bio - Intermolecular Attractions

Oil and Water Shaken Up and Mixed



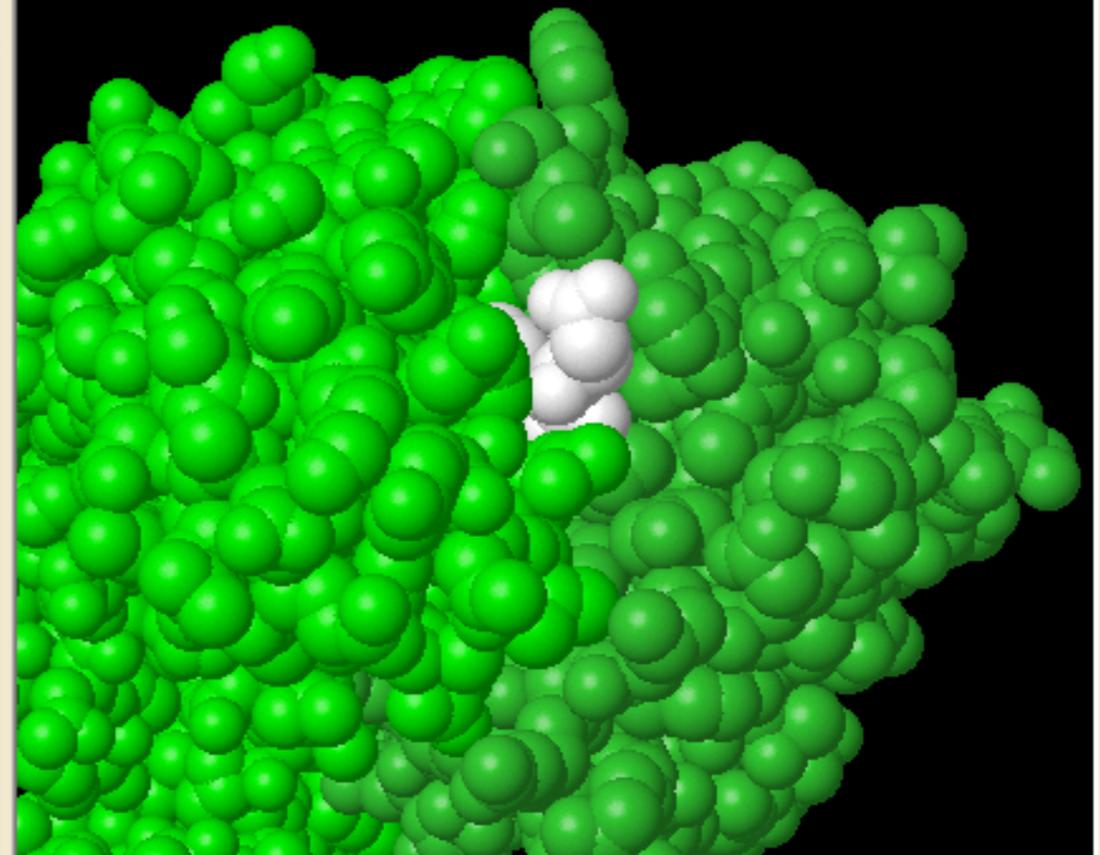
press run to see the mixture "settle"

▶ Run

⏸ Stop

⏪ Reset

Antibody/Antigen



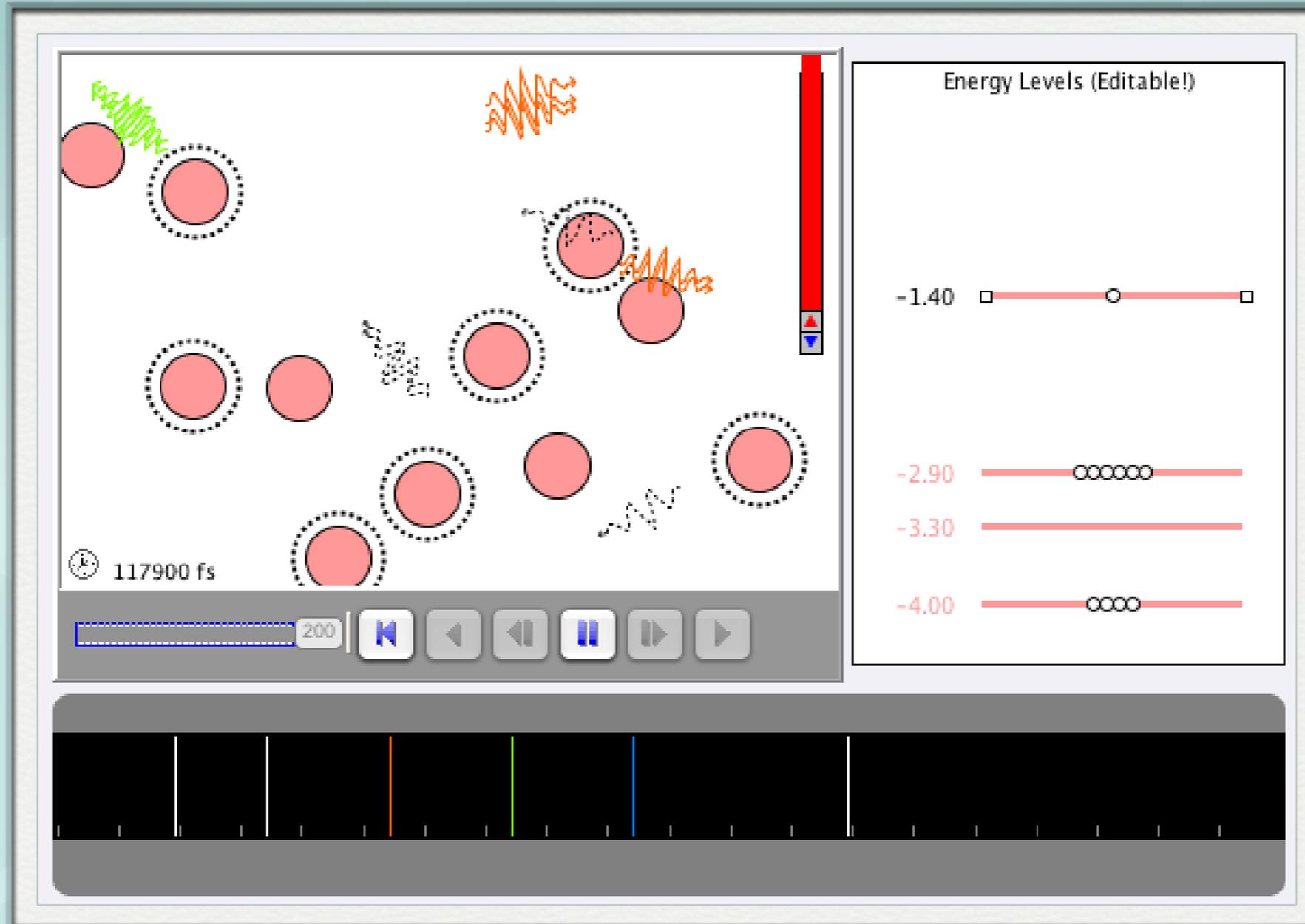
▶ Run

⏸ Stop

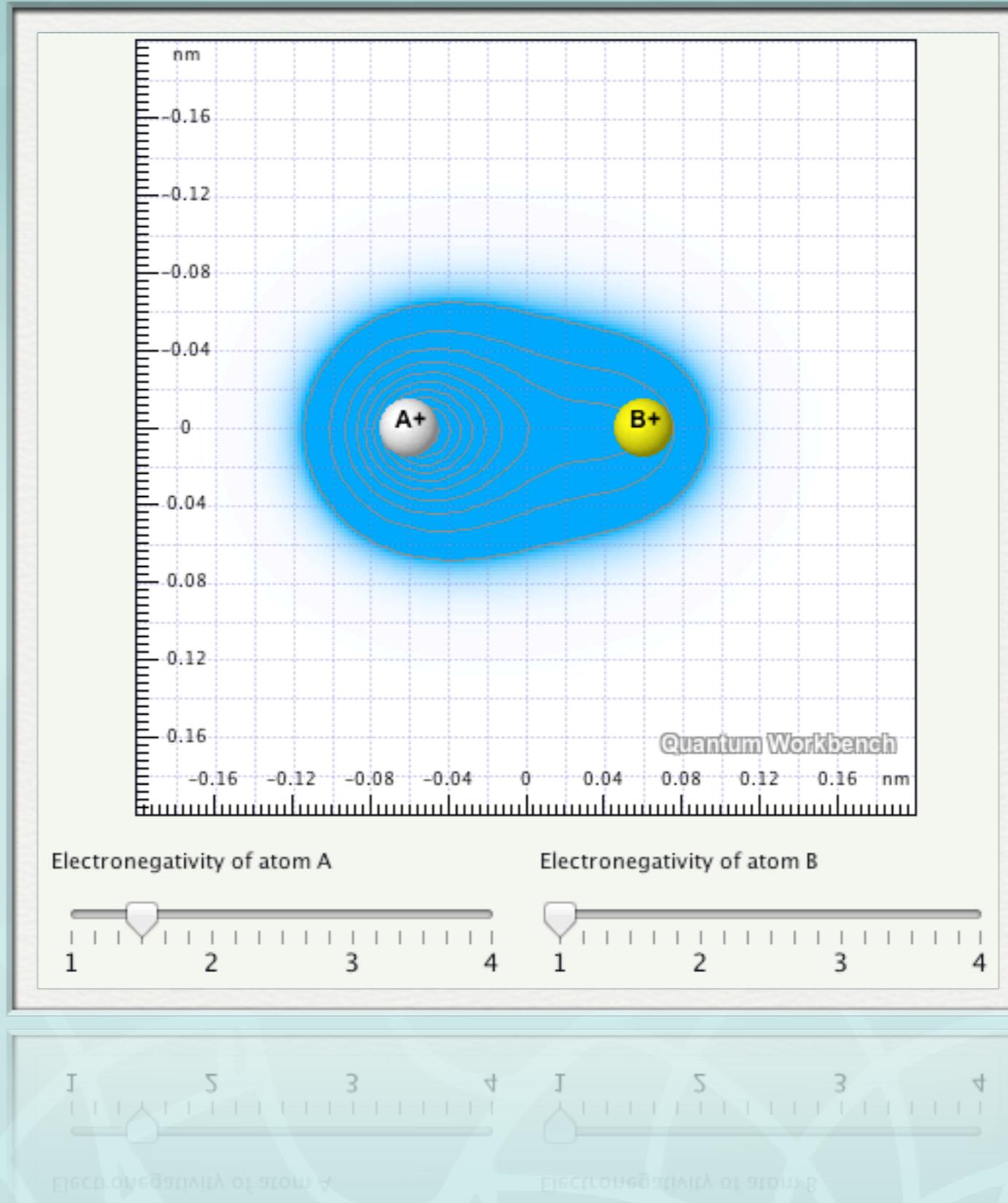
⏪ Reset

press run to see the mixture "settle"

Phys/Chem - Spectroscopy



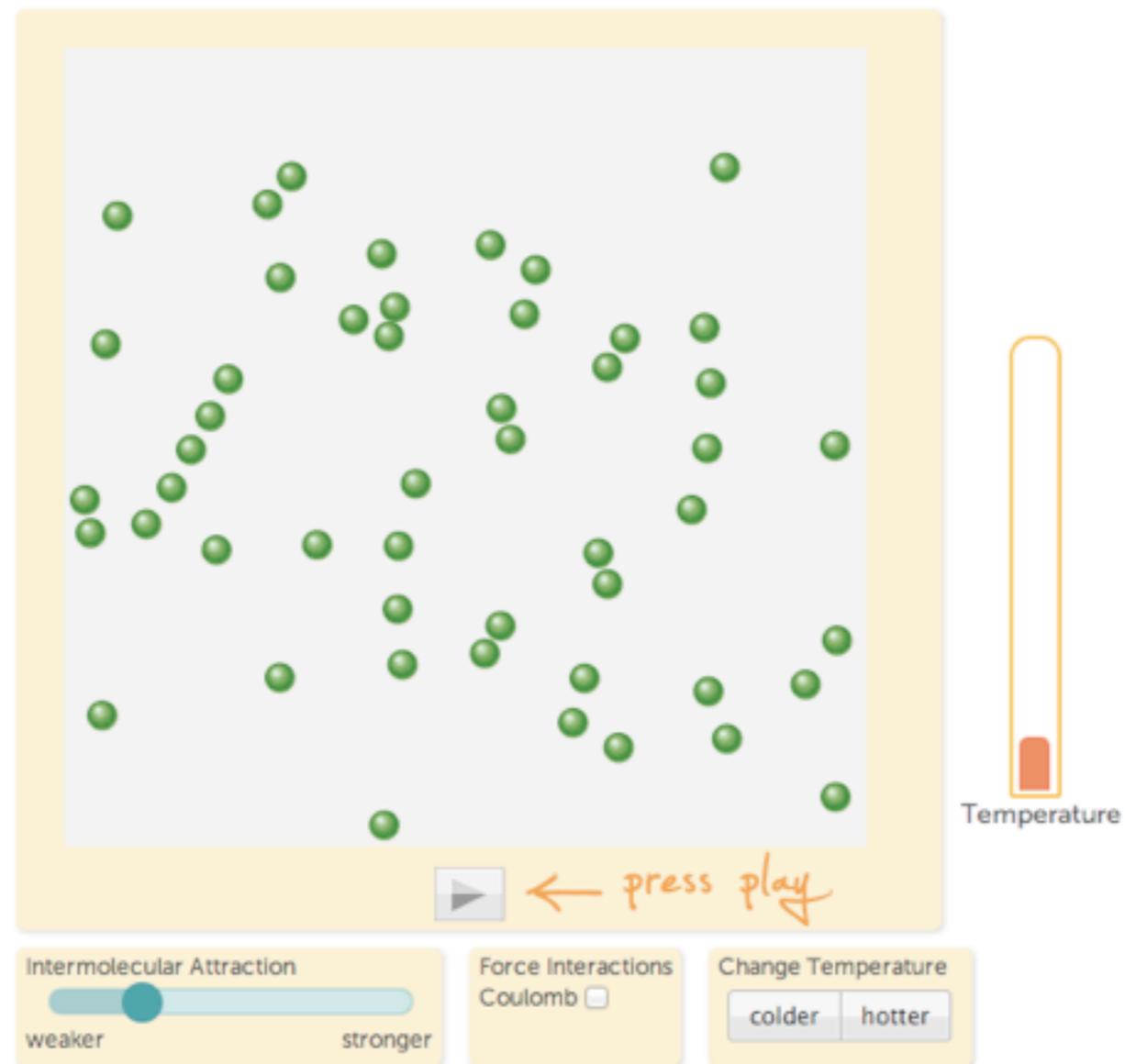
Quantum Chemistry - Polar Bonds



Switch to HTML5/ JavaScript

Atoms. In Your Browser.

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The screenshot shows a web-based molecular simulation interface. At the top, a large rectangular window displays a collection of green spheres representing atoms, some of which are clustered together. Below this window is a control panel with three main sections: 1) 'Intermolecular Attraction' with a horizontal slider ranging from 'weaker' to 'stronger'; 2) 'Force Interactions' with a checkbox labeled 'Coulomb'; and 3) 'Change Temperature' with two buttons labeled 'colder' and 'hotter'. To the right of the simulation window is a vertical thermometer labeled 'Temperature' with a red liquid level. Below the simulation window, there is a play button icon and the handwritten text 'press play' with an arrow pointing to the play button.

Benefits of the Web Platform



Molecular Workbench
Visual Interactive Simulations for Teaching & Learning Science



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States of Matter

How does the particulate nature of matter help explain the different states of matter?

Matter is anything that has mass and occupies space. Matter is found in four different states: solid, liquid, gas and plasma. Each of these states is known as a phase. Explore the relationship between the atoms and molecules and the macroscopic properties of the different states of matter.

Explore the Model

- Click the play button.
- Use the slider to adjust the intermolecular attractions.
- Turn on Coulomb forces by clicking the box.
- Change temperature by clicking on the heating and cooling buttons.

Question 1 of 4
How many atoms appear in the model?

1

50

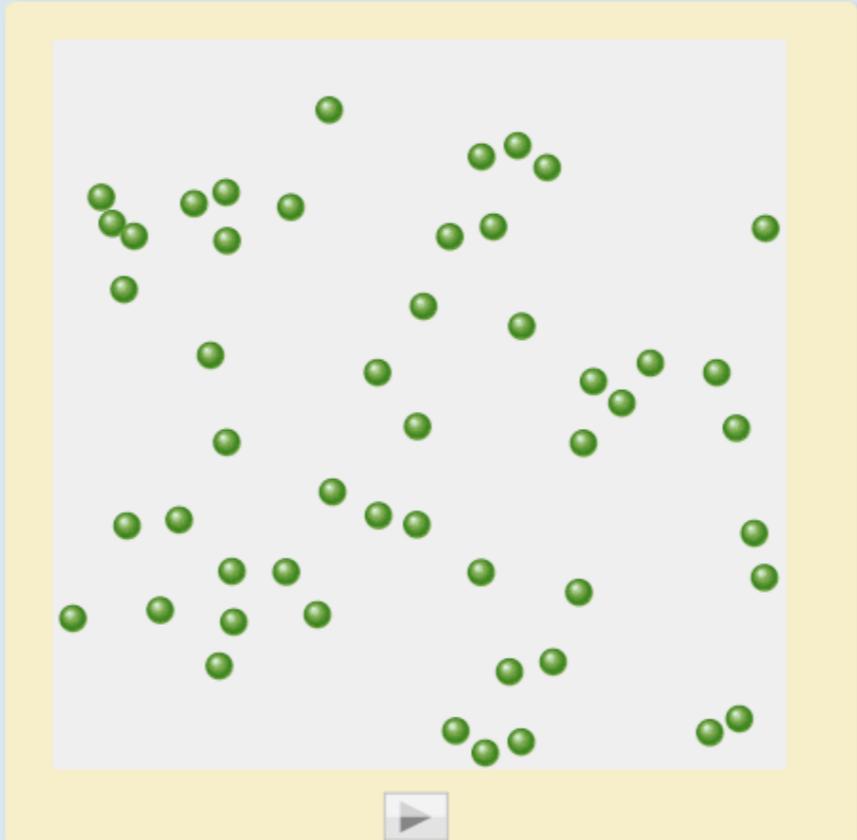
1000

9

Check Answer

Next

Embed | Share | Full Screen



Temperature

Intermolecular Attraction
weaker stronger

Force Interactions
Coulomb

Change Temperature
colder hotter

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Inquiry Is Key

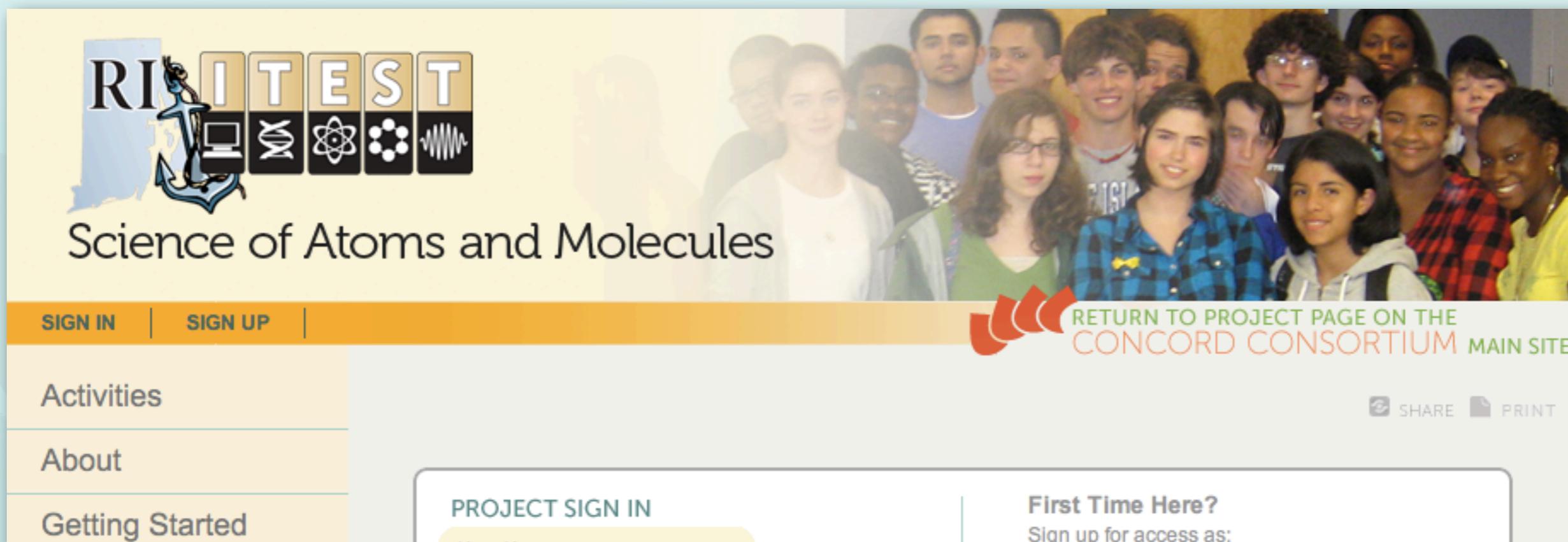
- Going deeper can simplify science
 - Most scientific phenomena can be explained by fundamental ideas of the atomic nature of matter, conservation of energy, Nature's tendency toward equilibrium.
 - Science through this lens is more connected - less individual facts to "memorize".
- Conceptual understanding is the goal.
- Utilize interactive models, to allow inquiry at the atomic level.
- Teachers are essential for inquiry approach to work.

Finding Materials

- **Molecular Workbench Application and Database**
<http://mw.concord.org>
- **NextGen MW - HTML5 version**
<http://mw.concord.org/nextgen/>
- **Various Project portals**
<http://www.concord.org/projects>

Previewing Models and Using the Portal

- Go to: <http://ri-itest.portal.concord.org>
- or <http://et.portal.concord.org>
- Click on the “Activities” link.
- Click the  button on an activity.



The screenshot shows the RI-ITEST portal website. At the top left is the RI-ITEST logo, which includes the letters 'RI-ITEST' and icons for a computer, DNA, an atom, a molecular structure, and a waveform. Below the logo is the text 'Science of Atoms and Molecules'. To the right of the logo is a large group photo of diverse students. Below the photo is a navigation bar with 'SIGN IN' and 'SIGN UP' buttons. To the right of the navigation bar is a red arrow icon and the text 'RETURN TO PROJECT PAGE ON THE CONCORD CONSORTIUM MAIN SITE'. Below the navigation bar is a sidebar with 'Activities', 'About', and 'Getting Started' links. At the bottom of the page, there is a 'PROJECT SIGN IN' button and a 'First Time Here?' section with the text 'Sign up for access as:'.



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