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Learning Chemistry through Inquiry: the Molecular Workbench to the Rescue

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According to the National Science Education Standards [1], "inquiry into authentic questions generated from student experiences is the central strategy for teaching science." Inquiry involves asking and investigating questions, gathering and analyzing data, and predicting and explaining results. Because of its experimental nature, inquiry is typically taught through hands-on activities.

But atoms and molecules, the core idea in chemistry, are too small to be touched by bare hands. The conceptual abstraction of atoms and molecules and their motion and interaction often leaves instructors few options other than teaching them as facts.

The *Molecular Workbench* (MW) software (http://mw.concord.org) is a computational modeling system that can be used to support inquiry into the molecular world [2]. MW simulations generate dynamic visualizations of microscopic processes that can be observed, manipulated, and analyzed on the computer screen. This simulation capacity offers a powerful means of experiential learning in the absence of direct hands-on opportunities. MW offers completely visual learning experience, which allows the majority of students to learn about the concepts and ideas in atomic-scale science without being bogged down in the difficulty of mathematical and technical details.

The computational engines of MW for simulating molecular motions and quantum waves grew out of contemporary molecular modeling research [3]. As such, MW is not just an animation tool. It has all the predictive and explanatory power delivered by the research-grade computational methods built in it. That power is fundamentally important to enabling "digital inquiry." If we agree on the parallelism between inquiry in science and inquiry in education, why not give students a research tool and make it easy enough for them to use?

One of the concerns from teachers about using professional-grade computational tools in classrooms is that they tend to have complex functionalities for tackling complex relationships. This kind of complexity is often overwhelming to students. MW addresses this issue by introducing a user interface builder that allows curriculum designers to make custom controls for a specific simulation. These controls provide simple, direct user interactions with a simulation and set up a "sandbox" to confine student exploration within a subject. Within this "sandbox," students can investigate one variable at a time.

In his Foreword for a National Research Council's report on inquiry-based learning, Bruce Alberts singled out an important inquiry skill: "One skill that all students should acquire through their science education is the ability to conduct an investigation where they keep everything else constant while changing a single variable. This ability provides a powerful general strategy for solving many problems encountered in the workplace and in everyday life."[4] In many hands-on activities in chemistry labs, however, it is not always easy to find two substances that differ in only one property or vary just one property of a substance at a time. But this is not a problem for a computer simulation.

To be concrete about how this kind of inquiry is made possible in MW, let's look at a couple of examples that chemistry teachers typically teach and discuss how computer simulation can transform our teaching practices. These simulations may be commonplace to some readers. But they provide a good starting point to initiate a discussion.

A phase simulation lab

When learning states of matter, students are often taught in a way as if the three states, gas, liquid, and solid, were separate things. But, in fact, the formation of a phase is determined by only a few factors that are common to materials in any state made of any kind of atoms. An MW simulation shown in Figure 1 was designed for students to discover whether or not they can "cause a phase change" by adjusting one variable at a time. Students can explore four independent variables: atomic mass, atomic radius, interatomic attraction, and temperature. Using the simulation, students will be able to assess the effect of each individual variable. Those that do not have a significant role on phase change are used as distracters that can be ruled out through inquiry.

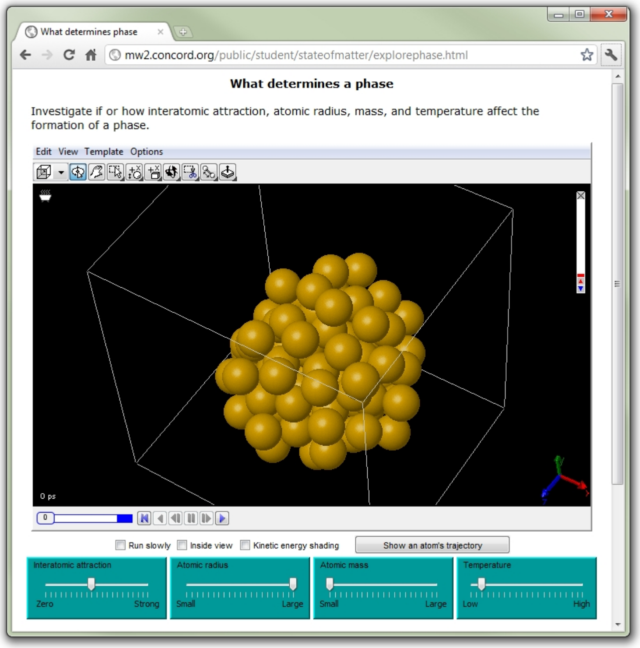

Figure 1. An online molecular dynamics simulation that students can use to investigate if or how interatomic attraction, atomic radius, mass and temperature affect the formation of phases.

Students can also study how the variables are correlated. For instance, they may find out that the melting point of a solid can be increased by making the attraction among the particles stronger. They can investigate whether substances made of larger or more massive atoms would necessarily have a higher melting or boiling point. This permits teachers to pose questions such as why mercury is a liquid and radon is gas whereas aluminum is solid.

The opportunities of inquiry provided by this simulation would hardly be possible if the molecular dynamics technique had not been used to construct it. Although molecular dynamics is based on only a few fundamental rules that connect the above four variables, it is capable of producing many different emergent behaviors and rendering countless subtle details. The details can further enrich the inquiry experience and lead students to deeper exploration. For example, students can randomly pick a particle and trace its trajectory. They can compare the trajectories of particles in different states. These manipulations of the simulation provide students much more learning opportunities than just telling them how atoms move in different states as many textbooks currently do.

A gas simulation lab

Everyone teaches the Ideal Gas Law. An ideal gas is a hypothetical gas made of randomly moving particles that do not have a volume and do not interact with each other. Have your students ever asked questions such as “What about non-ideal gases? How good is the Ideal Gas Law for real gases?” To answer those questions, you probably would have to pull out the Van der Waals Equation and pray that doing the math would do the trick.

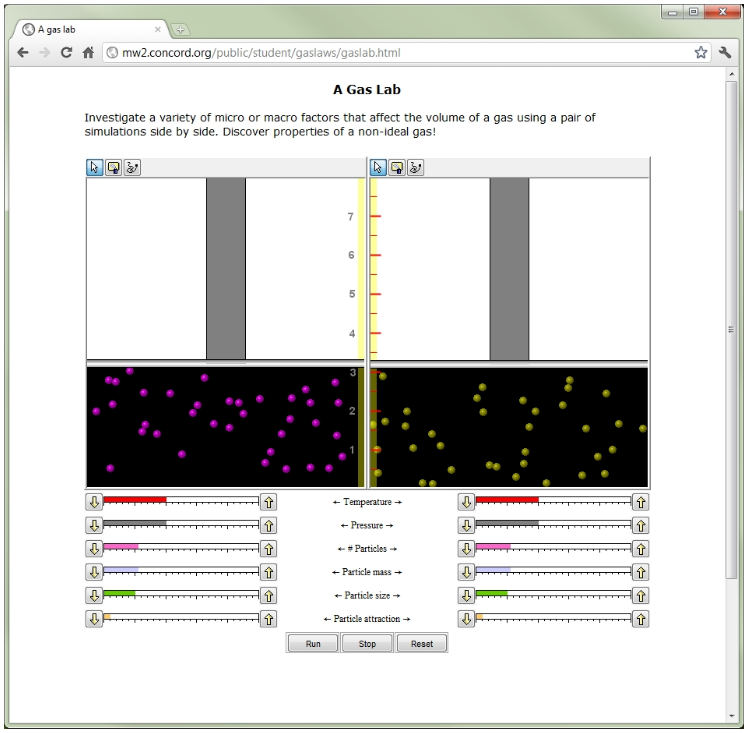

Figure 2. An online molecular dynamics simulation that students can use to investigate how well the Ideal Gas Law approximates real gasses.

Now, there is a better way to teach this. Using an MW simulation shown in Figure 2, investigating non-ideal gases becomes a piece of cake. This simulation uses a pair of gas containers side by side and allows the user to explore if or how six variables affect the volume of a gas: temperature, pressure, number of particles, particle mass, particle size, and particle attraction. It basically covers all the variables in the Van der Waals equation—without saying them explicitly. And there is a variable that is not included in the Van der Waals equation. The simulation reveals exactly why it is not there.

It is noteworthy that this simulation uses a setup of two gas containers that makes it easy for students to compare the results whenever they modify a variable for one gas.

A final note

The Molecular Workbench software has many more existing simulations that cover many topics in science. And best of all, if you are not satisfied with one, you can create your own.

References:

[1] National Research Council, *National Science Education Standards*. Washington, DC: National Academy Press, 1996.

[2] C. Xie, R. F. Tinker, B. Tinker, A. Pallant, D. Damelin, and B. Berenfeld, "Computational Experiments for Science Education," *Science,* vol. 332, pp. 1516-1517, 2011.

[3] A. R. Leach, *Molecular Modeling: Principles and Applications*, 2nd ed.: Pearson Education, 2001.

[4] National Research Council, *Inquiry and the National Science Education Standards*. Washington, DC: National Academy Press, 2000.

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fig1p4fall2011cccenl.jpg	281.73 KB
fig2p4fall2011cccenl.jpg	262.62 KB