THE CONCORD CONSORTIUM PRESENTS

THE MOLECULAR WORKBENCH

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National Science Foundation
WHERE DISCOVERIES BEGIN

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THE CONCORD CONSORTIUM

Realizing the Promise of Educational Technology

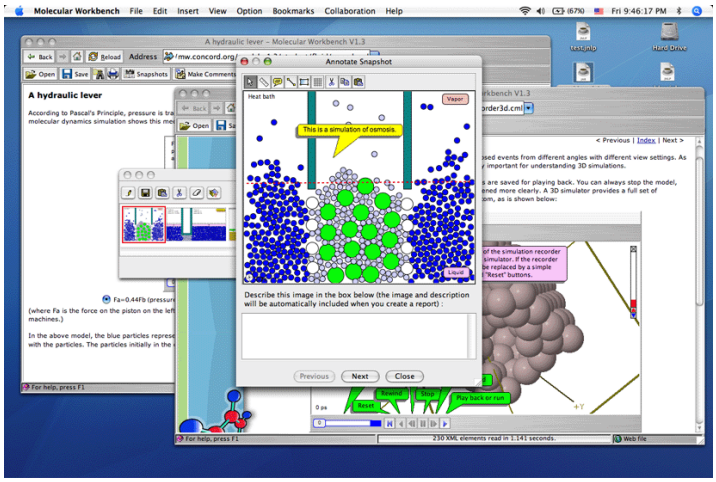
www.concord.org

The Concord Consortium is a nonprofit educational research and development organization based in Concord, Massachusetts. We create interactive materials that exploit the power of information technologies. Our primary goal in all our work is *digital equity* — improving learning opportunities for all students.

The Concord Consortium

Introduction

The Molecular Workbench is a free, open-source software package for creating and delivering interactive scientific simulations and learning modules based on these simulations. Students can experiment with atomic-scale systems to understand a wide variety of concepts such as the kinetic molecular theory, gas laws, diffusion, heat transfer, phase change, chemical reactions, fluid mechanics, material properties, structure-function relationships, genetic code, protein synthesis, light-matter interactions, quantum phenomena, and much more.



The Molecular Workbench on Mac OS X. This image shows a snapshot from a simulation of osmotic pressure. Students can annotate snapshots to capture what they observe or create.

With the Molecular Workbench, teachers and faculty can

- Use simulations to demonstrate concepts and enrich your lectures.
- Use curriculum modules published in the Molecular Workbench.
- Track student learning progress across curriculum modules.
- Design simulations and curriculum materials for teaching.
- Challenge students to create their own simulations to solve problems.
- Study how effectively computer simulations can help students learn.

> "These days, the first thing I do when preparing a lecture is to scour the Molecular Workbench for useful animations. I find animated simulations in general, and Molecular Workbench in particular, invaluable in bringing across complex concepts."
>
> *— Jan Jensen, Department of Chemistry, The University of Copenhagen*

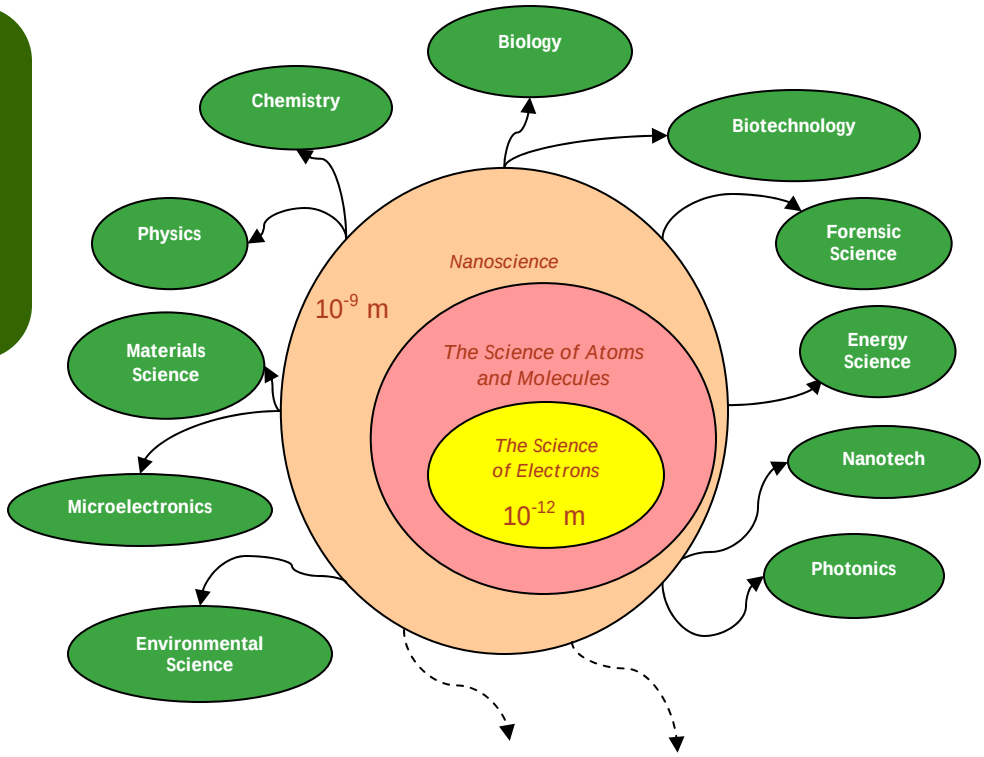
From middle schools to colleges, students all over the world use the Molecular Workbench to learn science.

Teaching atomic-scale science

"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, Nobel laureate

The science of electrons, atoms, and molecules (SEAM) is the foundation of modern science and technology.



New sciences—for example, nanoscience, energy science, and environmental science—increasingly draw upon **the science of electrons, atoms, and molecules (SEAM)**. Not only is it critical to scientists and engineers, but it is important to the scientific and technical literacy of the general public.

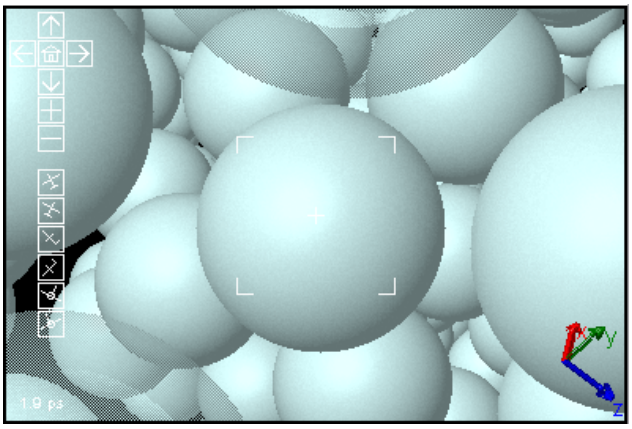
Teaching SEAM, however, can be a challenge. The atomic-scale world is alien to students: electrons, atoms, and molecules are tiny; they move fast; their interactions resemble nothing we see in everyday life; and their behaviors are complex and sometimes counter-intuitive. This is the world in which thermodynamics and quantum mechanics govern. Science education must address these learning difficulties head-on.

Teaching the science of electrons, atoms, and molecules is difficult because students lack intuition.

Computer simulation to the rescue

Visualizing microscopic processes

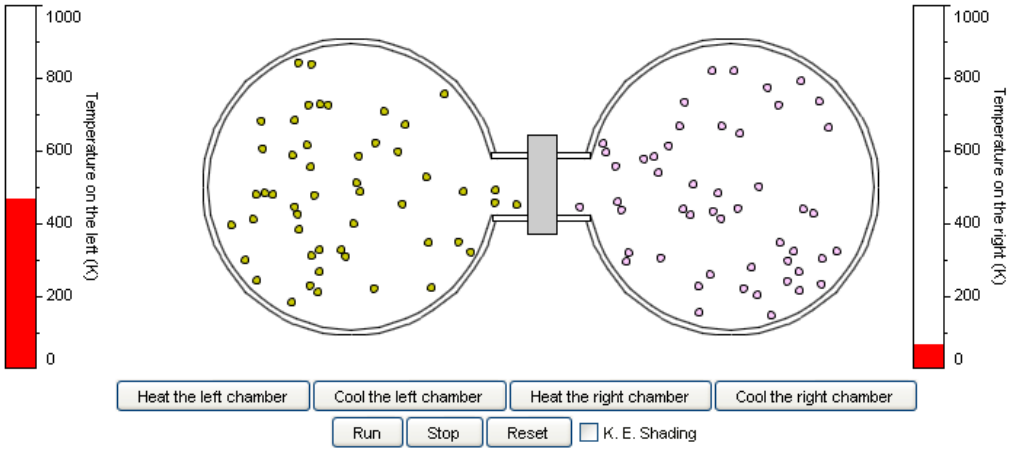
Individual electrons, atoms, and molecules are too small to be seen or touched. The Molecular Workbench helps students visualize what microscopic structures may look like and how they may move.



A view of atomic motion inside a liquid. The 3D simulator in the Molecular Workbench allows students to "navigate" into the world of atoms and molecules and select an atom to "ride." This feature allows students to experience the thermal motion resulting from random collisions.

Experimenting with simulations

The Molecular Workbench can be used to create interactive simulations that allow students to learn through manipulating variables and testing different "what-if" conditions. Hundreds of these simulations are available. By observing changes, students gain insights into the relationships among the variables and conditions. Such virtual experiments are similar to real experiments carried out in a wet lab. But simulations provide useful visualizations and interactions that are sometimes not feasible in real experiments. Simulations thus complement wet labs.



This image shows a simulation of heat and mass transfer between two gas chambers. The setup is similar to that of a real experiment in a chemistry lab. With this simulation, students observe how equilibrium is established through diffusion and collision—two processes that are not easy to visualize in a real experiment.

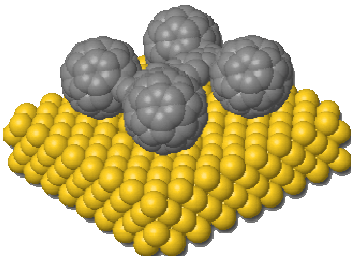
Simulations provide opportunities for students to explore, observe, discover, and learn.

Under the hood

How do Molecular Workbench simulations work?

The phenomena demonstrated by Molecular Workbench simulations are the result of sophisticated calculations based on fundamental equations from first principles in physics.

These equations are capable of simulating a large number of phenomena in physics, chemistry, and biology. But the capacity alone is not enough for building educationally useful simulations, which require high interactivity.



A molecular dynamics simulation of a nano car made of four C_{60} molecules.

The computational method used to simulate the motion of atoms and molecules is called the molecular dynamics method, which—in the classical case—is based on solving **Newton's equation of motion** for interacting particles:

$$m_i \ddot{\mathbf{R}}_i = -\nabla_i V(\mathbf{R}_1, \mathbf{R}_2, ..., \mathbf{R}_n)$$

where V is the potential energy function for the n interacting particles whose position vectors are represented by $\mathbf{R}_i$, m_i is the mass of the i-th particle, and the upside-down triangle is the gradient operator that computes the force on the i-th particle from the potential energy function.

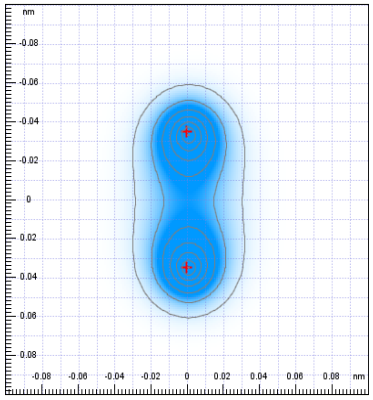
> "I am inspired by the biological phenomena in which chemical forces are used in repetitious fashion to produce all kinds of weird effects (one of which is the author)."
>
> — *Richard Feynman*

For students to be able to interact with simulations, the calculations in the Molecular Workbench are done in real time—quickly enough that students can experiment with many different situations within a short period of time. These real-time, interactive simulations have the potential of helping students develop solid conceptual understanding that is difficult to achieve using traditional curriculum materials.

The computational method used to simulate the motion of electrons is based on solving **the Schrödinger equation**:

$$i\hbar \frac{\partial}{\partial t}\psi(\mathbf{r},t) = -\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r},t) + V(\mathbf{r})\psi(\mathbf{r},t)$$

where $\psi(\mathbf{r}, t)$ is the wave function, $V(\mathbf{r})$ is the potential energy function, m is the mass, and $\hbar$ is the Planck constant.



A quantum dynamics simulation showing the formation of a nonpolar covalent bond.

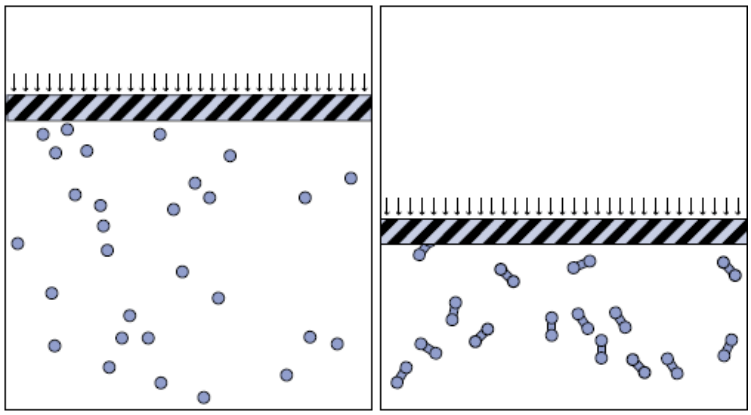
The best way to visualize science is to use science itself to build the visualizations.

Creating your own simulations

"Imagination is more important than knowledge." — *Albert Einstein*

The Molecular Workbench can be used to create new simulations. It is a user-friendly tool for students, teachers, and developers.

The Molecular Workbench opens up opportunities for **students** to learn by building their own simulations to answer a question or solve a problem. As students create simulations, they gain deeper insights into important concepts in science, how they are connected, and how to apply them to design working systems.



A simulation created by a student showing that the volume of a gas of 15 diatomic molecules is only half that of a gas of 30 atoms. The atoms in both containers have exactly the same properties, and the pressure, temperature, and pistons are identical. Running the two models side by side at the same time makes it easy to observe the differences of their emergent behaviors.

Three levels of using a simulation tool:

- **Students watch what happens in a simulation.**
- **Students interact with a simulation and observe the changes.**
- **Students build a simulation to solve a problem.**

According to the theory of constructionism, building a simulation is the most effective way of learning.

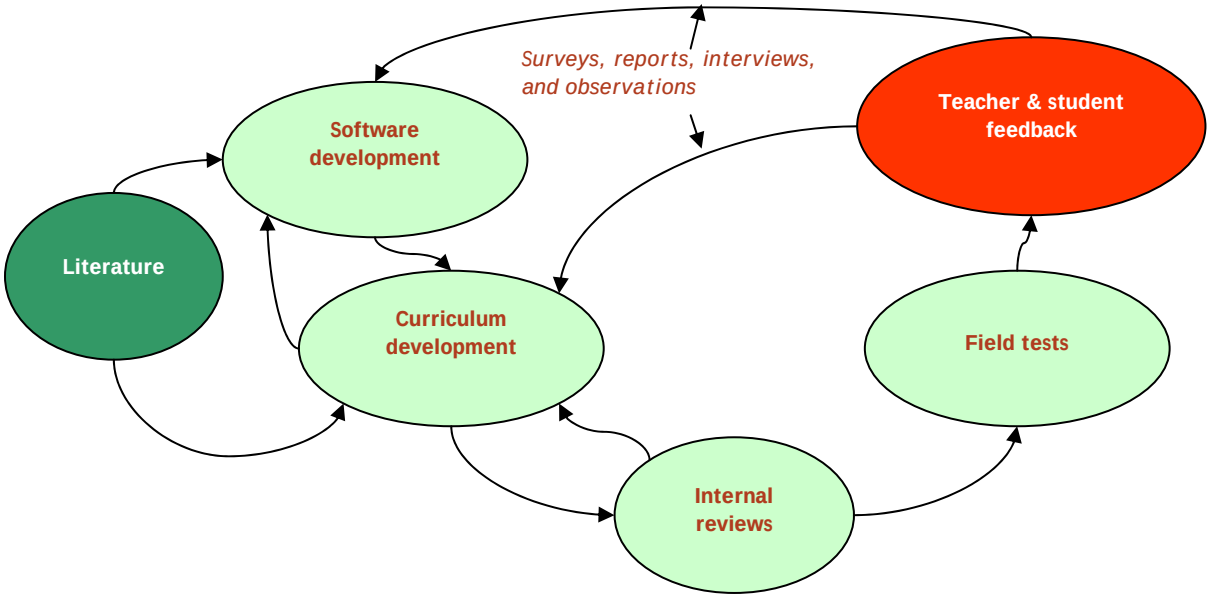
If you are a **teacher**, you may be interested in creating your own simulations—either based on existing ones or from scratch—to teach specific concepts. The Molecular Workbench also provides a curriculum authoring system with which you can use your simulations and develop full-fledged learning modules around them.

If you are an **educational media developer**, the computational engines in the Molecular Workbench free you from having to manually animate the motion behaviors of the phenomena you are interested in modeling. You can focus instead on configuring the structures, interactions, initial conditions, boundary conditions, and external inputs.

Conceptual understanding deepens when students build their own simulations.

Research-based curriculum development

The Concord Consortium and collaborators have produced dozens of learning modules. These modules have been field-tested and revised based on feedback from classrooms. The following diagram illustrates a typical development process.



Research studies have demonstrated that Molecular Workbench learning modules can result in student learning gains, transfer, and retention. One study showed that students could accurately and easily recall concepts learned two to six months after completing the activities. Pilot tests also indicated that students who were challenged to build their own models using the Molecular Workbench demonstrated a deepened conceptual understanding of fundamental science concepts.

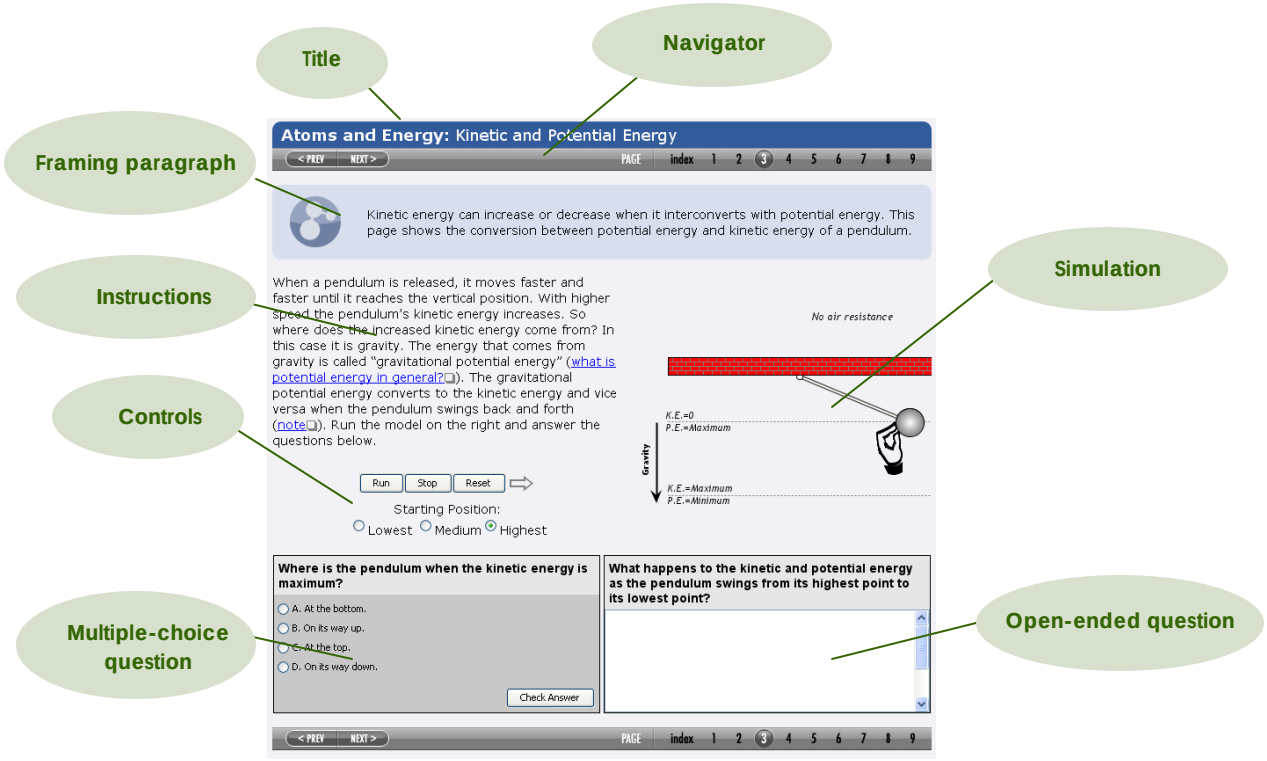
> "My experience with Molecular Workbench has been amazing. Using Molecular Workbench in my Physical Chemistry class, I was able to understand the dynamics of properties, systems, and processes visually. For instance, I was able to run experiments by setting up simulations and changing one property at a time. I think all Physics and Chemistry classes should use Molecular Workbench because it provides an alternative way to grasp concepts outside of just lecturing in the classroom. It allowed me to explore in a way unimaginable before when I built a fuel cell simulation step by step myself. I could let my curiosity flow by exploring how each editing tool affected my creation. I could also see other simulations built by students from around the world. Thus, I was able to learn in two ways—by attempting my own experiment and by analyzing other simulations."
>
> *— Britiany Sheard, student, Bowling Green State University*

Curriculum materials development at the Concord Consortium is driven by educational research.

Redefining textbooks

What will electronic textbooks look like in the future?

The Molecular Workbench delivers contextualized simulations through comprehensive learning modules. These modules contain scaffolded steps that include text, simulations, graphs, assessments, challenges, and networking capabilities. Students can answer questions, save their work in a web portfolio, share models with collaborators, create electronic reports, and submit them for grading. User interfaces can be customized for students of different levels, allowing a variety of pedagogical designs.

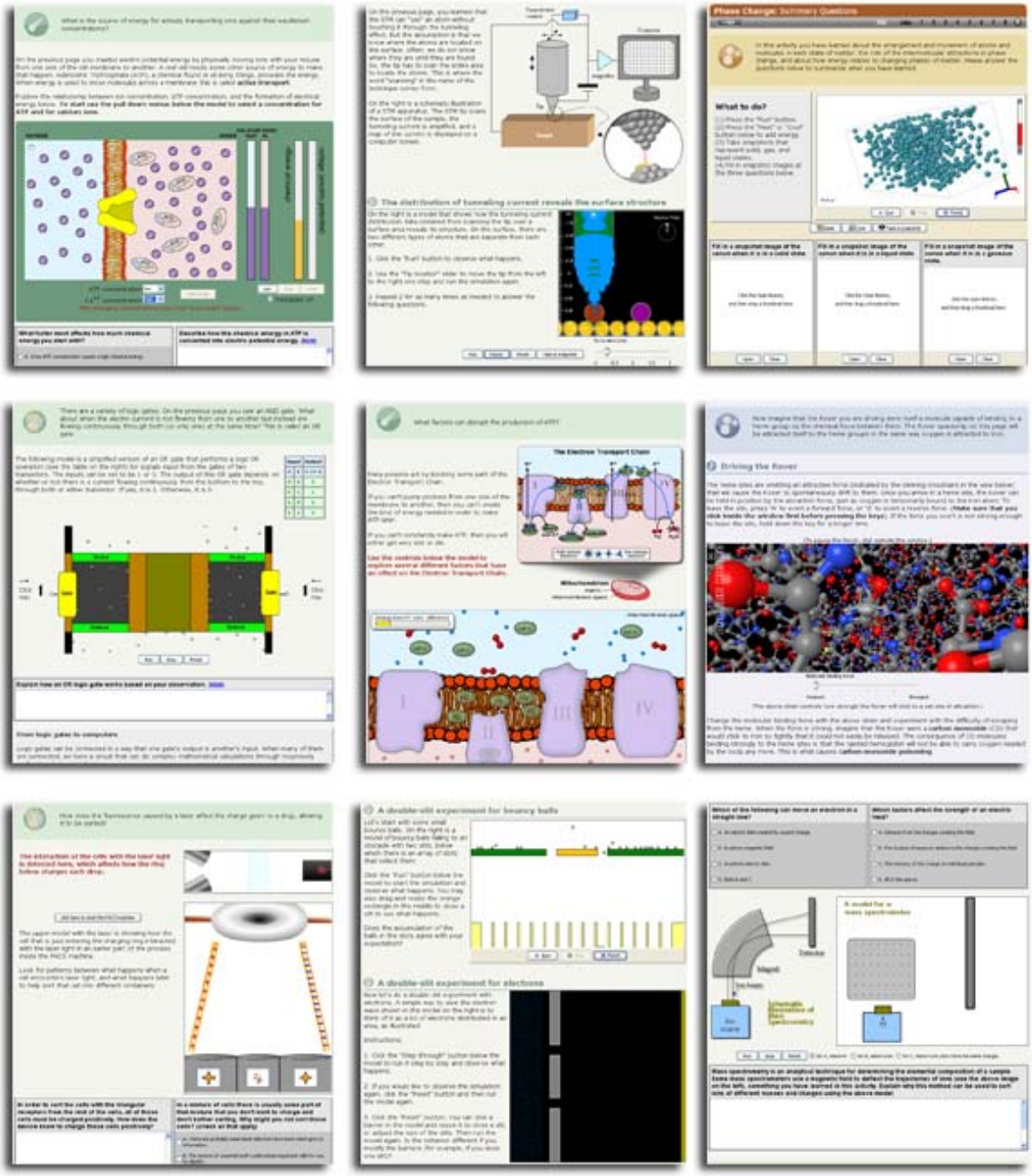


A sample Molecular Workbench page. Interactive simulations may be engines of future electronic textbooks.

A learning module in the Molecular Workbench is a prototype chapter in a next-generation electronic textbook in which interactive simulations replace static illustrations and student data are automatically collected and sent to teachers.

The next generation of electronic textbooks will replace static illustrations with interactive simulations.

Molecular Workbench curriculum



> "I LOVE the simulations and lessons that already exist in the Molecular Workbench family. They are easy enough to use even with someone as new as me." — *Teacher, Toronto, Canada*

Field-tested, classroom-ready curriculum materials are freely available in the Molecular Workbench.

Content coverage

The following curriculum modules are available in the Molecular Workbench.

Physics	Chemistry	Biology
Newton's Laws	Atomic structure	Diffusion
Heat and temperature	Kinetic molecular theory	Osmosis
Heat transfer	Gas laws	Active transport
Electromagnetic forces	Phase change	Cellular respiration
Electrostatics	Intermolecular interactions	Molecular recognition
Electrical conduction	Molecular geometry	Lipids
Semiconductors	Solubility	Carbohydrates
Quantum tunneling	Chemical bonding	Proteins
Double-slit diffraction	Chemical reactions	Nucleic acids
Excited states and photons	Catalysis	Genetic code
Photoelectric effect	Distillation	Transcription
Spectroscopy	Molecular crystals	Translation
Plasma	Polymerization	Photosynthesis

Biotechnology	Nanotechnology	Engineering
X-ray crystallography	Nanostructures	Transistor
DNA hybridization and Southern blot	Nanomachines	Fracture
ELISA	Self assembly	Hydraulics
Fluorescent tagging	Scanning tunneling microscopy	
FACS	Atomic layer chemical vapor deposition	
Electrophoresis	Sputtering	
Mass spectrometry		

More in the Molecular Workbench...

Broad content for grades 6-14.

Getting it to work in your school

Operating Systems	Windows 2000, Windows XP, Windows Vista, Windows 7, Mac OS X 10.4+, Linux
Memory	At least 128 MB
Required software	Java 5.0+ (downloadable from http://java.com)
Network connection*	Required for the online version.
Disk access*	Required for the online version.
Firewall*	The domain concord.org should not be blocked for the online version.
Proxy server*	For the online version, proxy can be set within the Molecular Workbench .

* These are not required if you use the offline version of Molecular Workbench included on the CD. However, the offline version does not have access to the latest materials and cannot be used to collect student data through the Internet.

Questions?

Contact:

Charles Xie

qxie@concord.org

The Concord Consortium

25 Love Lane

Concord, MA 01742

Phone: 978-405-3200

Fax: 978-405-2076

www.concord.org