Nanoscience and the New Secondary Science Curriculum

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"…a dramatic revision of the science curriculum can generate a truly revolutionary way of teaching science in U.S. high schools."– Leon Lederman, Nobel Laureate in Physics
"You mean there are air molecules hitting my arm all the time?" – 9th grader after having worked with a molec lar dynamics model.

Nanoscience and Introductory Science
Eric Drexler, the nanotechnology guru who coined the name "nanotechnology," summarizes the science content needed by students to understand nanotechnology as "molecular science." In his formulation, molecular science consists of "A knowledge of basic classical mechanics and electromagnetism is essential.. at least the rudiments of quantum mechanics…[and] knowledge of thermodynamics and of statistical mechanics." This represents a major change in science education, because in most curricula, mechanics is the only one of these four areas that is emphasized, and then not at the atomic and molecular level.

In addition, Drexler emphasizes chemistry, biochemistry, and engineering. Students should "seek at least a basic background in chemistry, focusing on its structural, molecular aspects … biochemistry is central: enzyme reaction mechanisms provide examples of what many nanomachines will need to do; the folding of proteins and the self-assembly of protein systems provide examples of how complex first generation molecular machines may be made." And "…one must learn to think as an engineer, and that means studying (and doing) design." Finally Drexler recommends paying "special attention to numerical simulation methods for molecular mechanical and quantum electronic systems" (Drexler, 1988).

No school would make such radical changes just to accommodate nanoscience. But, what is needed for nanoscience is needed across all of science education. The fact that nanoscience is not well served by the current science curriculum is a symptom that something wrong with the entire science curriculum. There is an equal problem faced by bioscience, electronics, photonics, systems engineering, and all the other interdisciplinary fields that have emerged in the last few decades. The problem is too much emphasis on formalism, too little emphasis on concepts, an outdated curriculum too focused on the disciplines, and a total lack of the science of atoms and molecules

Introductory science education needs a radical revision and nanoscience illustrates the new content that is needed. "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," says Leon Lederman, and, he contends, there is an urgent need to revise the introductory science curriculum to reflect this reality. Perhaps the best known alternative secondary science curriculum is "Physics First" (ARISE, 2001; Lederman, 1998, 2002; Lederman & Bardeen, 1998), which involves switching the secondary science sequence from biology-chemistry-physics to physics-chemistry-biology (PCB). The same goals can be accom-

plished with integrated science courses that span two or more grades, which are also gaining interest (e.g., California Science Teachers Association, 2006).

Yet attempts to revise the secondary science sequence generally involve simply re-arranging the sequence of topics without changing them. For instance, most PCB curricula offer a simplified traditional physics course followed by standard chemistry and biology courses. Without a new emphasis on atoms and molecules and the connections that this emphasis enables among the courses, there is little benefit to students. Most attempts to teach unified science (e.g., Bybee, 2006) fall into the same trap of reordering without adding the new science content needed. Without a deep treatment of atoms and molecules as a unifying theme, this kind of reordering will not significantly improve the science curriculum and can result in a net decrease of the quality.

The Missing Content

A solid set of materials that addresses atomic-scale science is the critical missing content needed to realize the dream of better introductory science curricula. The basic physics of atoms and molecules needs to be introduced early so that chemistry can take advantage of these concepts. Similarly, biology needs to leverage student understanding of atomic-scale physics and chemistry to address key introductory molecular biology concepts. This missing content represents only a fraction of each of the three courses. Biology, chemistry, and physics courses do not have to be re-written to profit from the new sequences. In most cases, the needed content can be substituted as an enhanced approach to traditional content.

It is in the context of increased emphasis on atoms and molecules that nanotechnology can be introduced naturally. Nanoscience itself cannot make a sufficiently strong case for its importance to change educators' thinking, but there is almost a perfect match between nanoscience and the concepts that are important to a unified atomic and molecular approach to the basic sciences. Thus, the need to include nanoscience in the curriculum helps justify the call for large-scale improvement in science education.

We are currently developing molecular science material that can be added to secondary science courses. On pages 8-10 below, we provide a summary of atomic- and nano-scale topics that be plan to add to physics, chemistry, and biology courses—eight for each course. These are organized into four thematic strands that span the three science courses when they are taught in the PCB sequence. In unified science sequences the content flow would have to be adjusted, but would have many of the same dependencies.

The strands—Motion and Energy, Atoms and Molecules, Charge, and Light—are based on fundamental concepts that can be introduced in the physics course and then elaborated and applied in chemistry. The resulting understanding of atomic and molecular science will enrich and deepen the subsequent treatment of biology. These topics have been selected to match the content sequences developed by the ARISE recommendations (Lederman, 1998) and developed through extensive consultation with teachers and administrators who are implementing PCB. These topics also match the content of Drexler's molecular science.

Each topic will be addressed in two or three class periods, so the new content will require 16-24 class periods for each of the three PCB courses. This is 10-15% of the available instructional time—enough to have an impact on learning but little enough to fit into existing courses. The content has been selected with the understanding that anything added to the curriculum forces out something. In each case, the proposed materials provide ways to teach traditional content, but from an atomic-scale perspective. For example, when studying 2D motion in physics, applications of Newton's laws to the motion of atoms can be investigated in place of other applications. This measured and carefully designed approach will simplify adoption— teachers will be able to keep their textbooks and introduce this new material gradually.

The Role of the Molecular Workbench

Computational models of the atomic world are essential to teaching atomic- and nano-scale science because they allow students to experience an otherwise inaccessible world and build mental models that can be used to understand and predict macroscopic phenomena. (Birk, 1997; Clark & Jorde, 2004; Hakerem, 1996; Stieff & Wilensky, 2002; Tinker, 2001a, 2001c, 2001d). Student explorations of these models can lead to a good understanding of connections between atomic-scale events and those events that they can observe at the macroscopic scale. (Berenfeld & Tinker, 2001; Buckley et al., 2004; Tinker, Berenfeld, & Tinker, 1999, 2000). Students can learn the atomic and molecular concepts that have been recommended for unified science or PCB curricula (California Science Teachers Association, 2006; Lederman, 1998).

There is only one computational model that can simulate all the phenomena that are included in the atomic- and nano-scale concept topics: the Molecular Workbench *(MW)*, an open source educational system based on molecular dynamics models that are used in research. The *Molecular Workbench* seamlessly integrates the following functions:

A set of molecular dynamics models and their associated input and output components.

An authoring system for constructing user interfaces to the models.

A word-processor for creating hypertext in which components of models can be manipulated.

An embedded assessment system that supports questions and collects student data.

A delivery system similar to a web browser.

Web services that support collaboration among authors.

The *Molecular Workbench* molecular dynamics simulations are based on the physics of atomic-scale interactions and can exhibit fundamental phenomena in physics, biology, and chemistry (Berenfeld & Tinker, 2001; Tinker, 2001b, 2001d). Simulations in *MW* calculate the motion of atoms, molecules, and other objects in real time as a result of the applicable forces, including the Lennard-Jones potentials, electrostatic potentials, elastic bonds, and external fields. Because it is based on good approximations of physical laws, *MW* can produce emergent phenomena such as phase changes, crystallization, latent heat, diffusion, solubility, osmosis, absorption, chemical equilibrium, catalysis, self-assembly, and biomolecule conformation.

Some novel features have been added to *MW* to handle computationally intense systems found at the nano-scale.

An effective field is used to model the hydrophobic and hydrophilic effects that influence protein folding.

Chemical bonds that have user-controlled energies can be made and broken to simulate chemical reactions (Xie & Tinker, 2006).

Large molecules can be created and charges added to them to simulate the interactions of large molecules (Berenfeld, Pallant, Tinker, Tinker, & Xie, 2004). This include Gay-Berne particles and "Smart Surfaces," described below.

Light-atom interactions are modeled with photons of selectable energy that interact with the excited states of atoms. Photons or thermal energy can excite an atom, which then can decay to a lower energy state by emitting a photon or generating kinetic energy. The excited states can be set by the user and the resulting spectrum of emitted photons can be observed.

3D. *MW* can now display 3D molecules, and there are already activities allowing students to interact easily with these molecules (e.g. from the Protein Database) and view component parts.

A *Molecular Rover* is currently under development that allows the user to 'move around' 3D molecules and experience local forces.

Gay-Berne Particles

A Gay-Berne particle is an approximation of a large molecule, such as found in liquid crystals, biological systems, and nano-engineering. These particles can be ellipsoidal generalizations of the atoms more commonly used in molecular dynamics. The two parameters of the Lennard-Jones potential are replaced by four parameters that control the size and attractive forces along two orthogonal axes. In addition, these particles can have charge and dipole moments. Fig. 1 illustrates how liquid crystals can be modeled using these particles

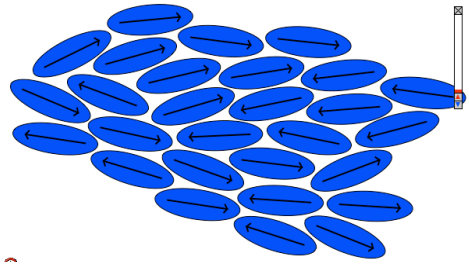


Figure 1: Nano-particles that self-attract and have dipole moments. These Gay-Berne particles are good approximations of liquid crystal molecules and can model a liquid crystal's response to temperature and electrical fields. [1]

Self Assembly

Self-assembly is a nano-engineering concept borrowed from biological systems. The underlying science of self-assembly includes the van der Waals force, Coulomb forces due to charged regions of molecules, and geometry. To build in the impact of shape, MW has "Smart Surfaces" that can be drawn by the user. These surfaces are actually chains of MW atoms linked together with elastic bonds and covered by a flexible surface that hides the atoms. Charge can be added to the periphery of a Smart

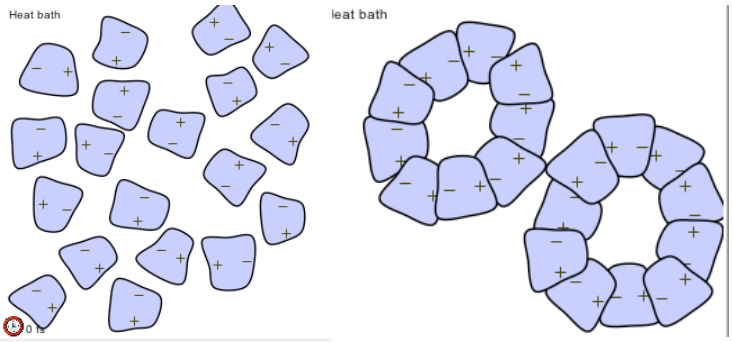


Figure 2. Self assembly. The smart surfaces on the left will self-assemble into the shapes on the right when the *MW* model is run. Students can create the surface shapes and determine

Surface. The result is a good approximation to a large molecule. It can hold its general shape, but it does vibrate, respond to temperature, and exert both long-range Coulomb forces as well as short-range attractive forces.

Smart Surfaces can be made to self-assemble. Fig. 2 is an example of a particularly interesting kind of self-assembling object based on nine identical sub-units. Fig. 3 demonstrates the importance of shape in docking, an effect that is similar to self-assembly. This model can be heated to separate the two molecules and then both the ball and triangle bounce around. On cooling, the triangle eventually finds its way back to the complementary surface through a random walk that takes quite a long time. This gives one an appreciation for the time-scale of molecular events of this type.

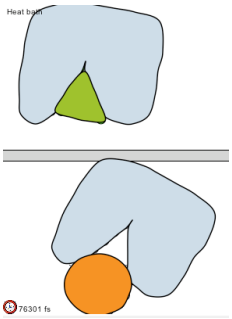


Figure 3. Docking. Students can discover that the upper complex is more robust and that the lower falls apart when heated.

Authoring in MW

The authoring functions built into *MW* can be used to create or modify student learning activities. The ease of creating *MW* materials has led to over 300 activities contributed by staff and collaborators. Many are housed in a database with fields that include an overview, learning objectives, a description of the central concepts addressed, textbook references, and extensions[1].

The illustrations on pp 11-12 show how a topic such as van der Waals forces can be treated using the *MW* authoring system by having students interact with a series of *MW* molecular dynamics models. The static pictures shown are a pale representation of the dynamic models, which can be explored by launching the activity at http://molo.concord.org/database/activities/227.html.

MW is written in Java, so it runs under Mac OSX, Windows, and Linux. It is open source, so it can be shared and copied by any user. International use of *MW* is growing; users from more than 60 countries have downloaded over 100K copies of the software and 500K copies of models and activities.

Molecular Workbench Research Findings

Overall gains. Student use of *MW*-based activities have resulted in overall increases in student understanding of atomic scale phenomena at high school and community college levels. Thirty classes analyzed, representing a cross-section of grade, level, and demographics, showed significant gains ($p<0.01$) on paired t-tests in pre/post -test analysis. In the community colleges the largest score increases were for questions related to interpreting results of a simulated lab procedure, problem-solving regarding unexpected results and applying molecular reasoning to understanding techniques.

Molecular reasoning. Students were able to transfer their understanding of atomic-scale phenomena to new situations and to reason about macroscopic phenomena on the basis of atomic-scale interactions. Using 10 sequential activities for biology helped high-school bi-

[1] The database of activities: http://molo.concord.org. More on the model: http://mw.concord.org/modeler

ology students achieve fluency in reasoning at the atomic scale. Results from testing in 24 classrooms indicate that students can use these materials to develop robust mental models about intermolecular interactions and apply these to reasoning about biological phenomena. Molecular reasoning, as measured by the accurate use of atomic-scale reasoning in essays, increased from 15% to 57%.

A controlled experiment was carried out to test the effects of models on learning outcomes using an activity on the forces affecting protein folding. Students in the experimental condition received the activity with models. Students in the control condition received a well-designed and fully illustrated substitute that did not use computational models. Identical pre- and post-tests were given. All students improved, but the treatment group showed greater gains in the more difficult questions that required immersive visualization and prediction of the next model states.

Nanotechnology with MW

Nanomachines of various kinds can be constructed using MW[2]. For example, fig. 4 shows two investigations that are taken from MW activities that are currently under development. The vapor deposition activity closely models epitaxial growth from a vapor stage, including the possible imperfections that can be avoided by careful procedure. The right-hand machine is a pure fantasy, showing what a molecular machine might look like. It is a good lesson because it does show the pervasive nature thermal motion, and because the operation of the sorter depends on getting atomic properties right and how mechanical motion might grab and release atoms in a thermal environment. A wide range of nano-machines and fabrication models like these can be created with MW and embedded into interesting activities.

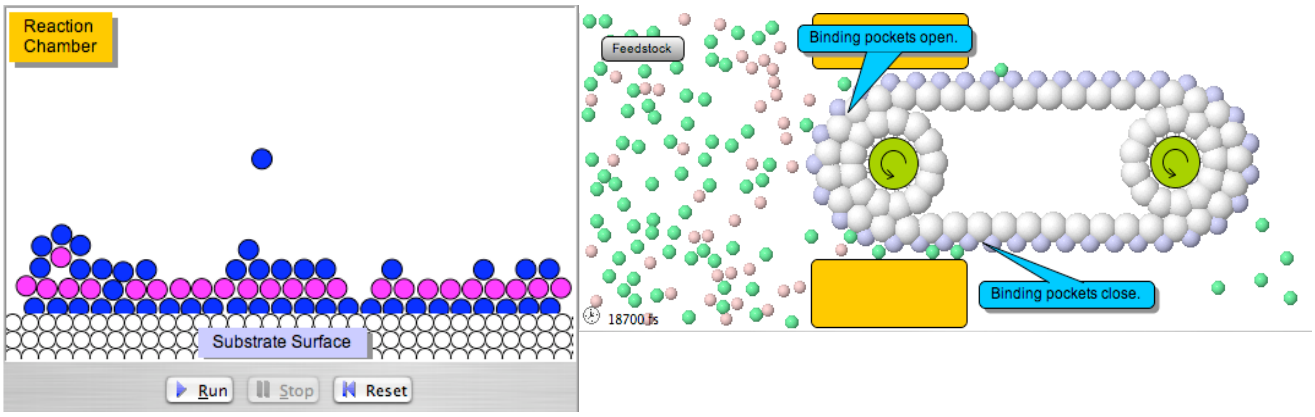


Figure 4. Examples of nanotechnologies modeled in the Molecular Workbench. On the left is a snapshot of a vapor deposition experiment with some atomic-scale imperfections. On the right is a nano-scale atom sorter. In the model, the tread rotates and van der Waals forces attract the green atoms into the slots, but not the red ones. The captured green atoms are released when the belt slots open up and eject the green atoms.

Three Dimensions

[2] For a library of them, go to http://mw.concord.org, click on "this link" about half way down the page. This loads MW and its index page. Go to the "library of models" and look for nanotechnology.

We are now adding “Rover” to the Molecular Workbench: a full set of 3D tools and visualizations that increase the nanoscience possibilities. Rover allows users to maneuver their perspectives and interact with moving molecular systems. As they do this, they can sense the local forces and see atomic motion.

The system includes three modules that allow educators to design interactive 3D activities. The first module is a WYSIWYG molecular constructor that allows educators to rapidly sketch up 3D virtual molecular worlds for student exploration (see Fig 5). The second is an interactive molecular dynamics simulation engine (see Fig 6). The third is a navigation engine that allows educators to decide the vista points of the constructed virtual worlds and the routes on which students will be guided to learn (see Fig. 7). The 3D graphics is rendered by using the Jmol graphics library. The entire system is seamlessly integrated with the Molecular Workbench (MW) software. This integration allows researchers to make use of the basic services MW provides, such as authoring, web delivery, embedded assessment, data mining, and user collaboration.

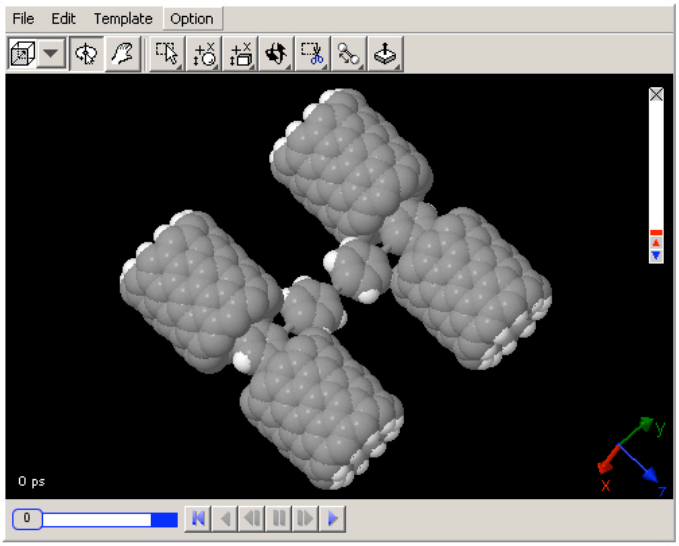


Figure 5: A nano car constructed using Rover’s 3D constructor.

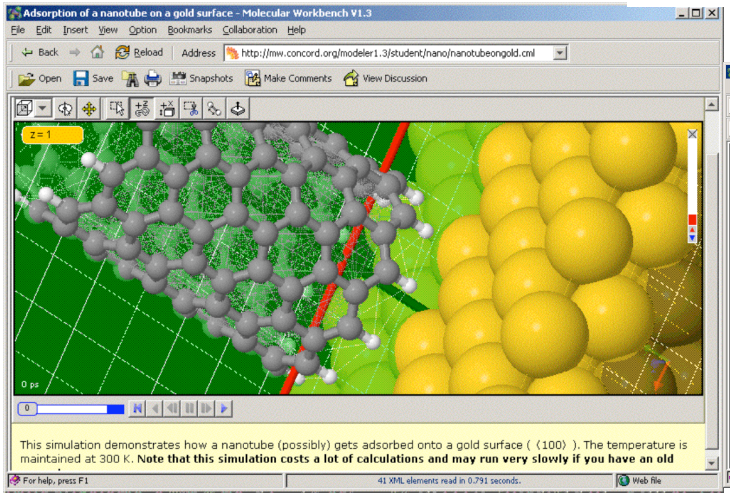


Figure 6: The inner window of this image shows a 3D construction scene for a model consisting of a gold surface and a carbon nanotube. The outer window shows that the 3D system is entirely integrated with the popular Molecular Workbench software.

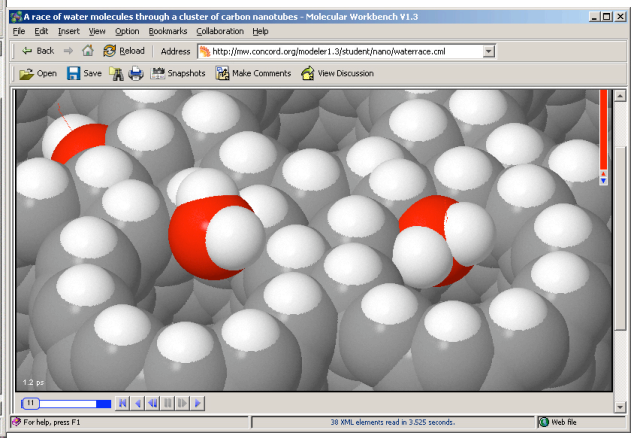


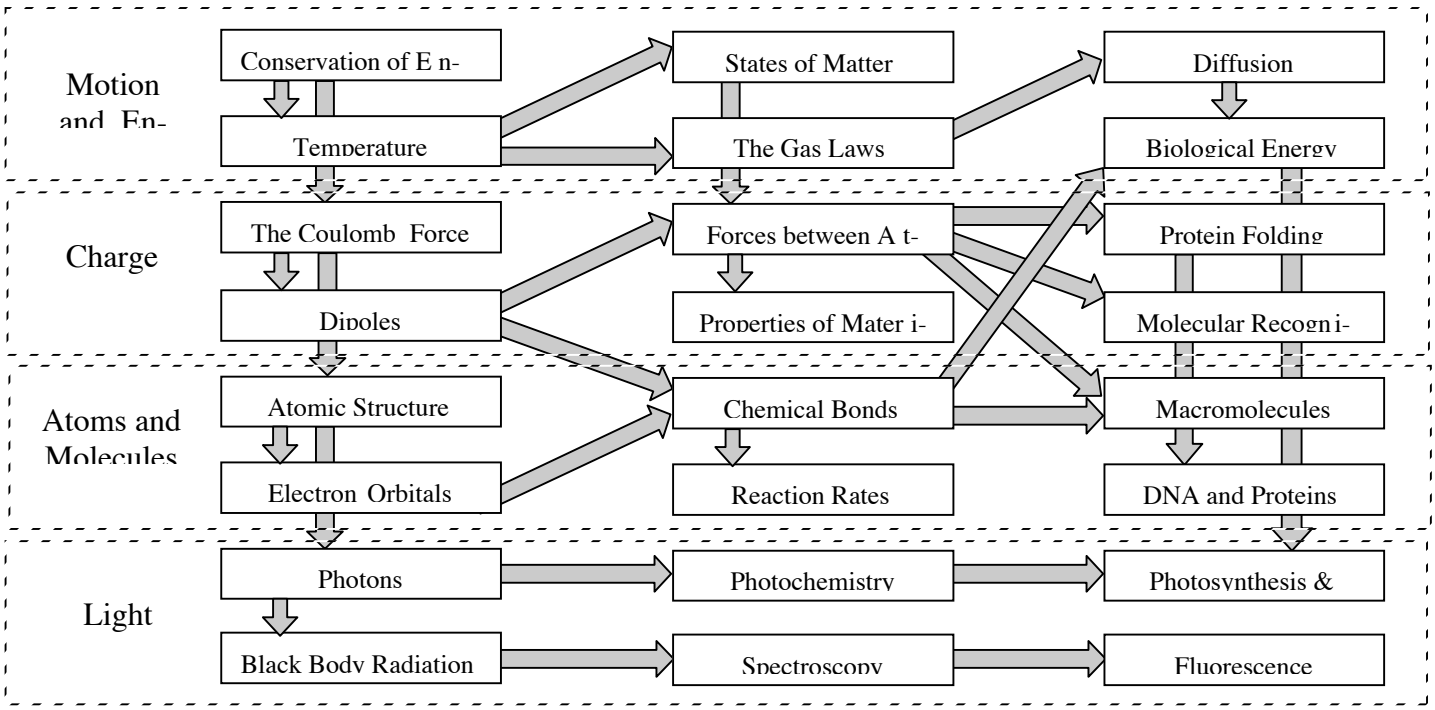
Figure 7: This image shows that during a molecular dynamics simulation, the user can “rove” into the 3D scene to observe the details. Here you see how water molecules make their way into carbon nanotubes.

Summary
Nanoscience is not going to be widely incorporated in science education until it can be seen as solving a problem, not just adding new content. The problem that is solves is to improve science education through the addition of the atomic and molecular science that is missing in biology, chemistry, and physics curricula, so, the needs of nanoscience education and science education intersect. Both require a basic conceptual understanding of atomic and molecular science. Good science education requires students to learn through inquiry by interacting with the systems being studied. At the nano-scale, the Molecular Workbench provides a unique tool for learning. It is a sophisticated, stable, and extensible system for creating and delivering inquiry learning activities in nanoscience based on guided student investigations.

Atom- and Nano-scale Concepts in Introductory Science

PHYSICS	CHEMISTRY	BIOLOGY
Motion and Energy		
E1. Conservation of Energy: The relationships and exchanges between force, motion, kinetic energy, and potential energy in atomic systems. Introduction of the van der Waals force and potential.	**E3. States of Matter:** Phases of matter, and the energy changes between states. (Condensation, latent heat, and inter-atomic potential energy).	**E5. Diffusion:** Thermal motion of biological molecules explains the molecular basis of diffusion and osmosis, life's temperature optimum, concentration gradients, and passive transport of materials across cell membranes.
E2. Temperature: Temperature is a measure of the average kinetic energy. At equilibrium all particles have the same average kinetic energy regardless of size, shape, or mass.	**E4. The Gas Laws:** Pressure is exerted through atomic collisions. Gas laws are derived from P, V, and T held constant.	**E6. Biological Energy:** Energy and the overcoming of disorder in biological systems. Applications will include ion gradients that produce voltage differences and the hydrolysis of ATP to ADP + P.
Charge		
C1. The Coulomb Force: The Coulomb potential energy, with electron-volt the appropriate atomic-scale energy unit.	**C3. Forces between Atoms and Molecules:** The various van der Waals forces among ions and dipoles, dipoles generated by fluctuations and induction and Hydrogen bonds.	**C5. Protein-Folding:** Amino acid characterization, and the affect on protein shape of solvent type (energy minimization).
C2. Dipoles: Magnitudes of electrostatic forces among charges and dipoles at the atomic scale. (Induction and induced dipoles, capacitors and electrometers).	**C4. Properties of Materials:** The atomic basis of a range of macroscopic properties of materials, including melting and boiling points, solubility, thermal expansion, and hardness.	**C6. Molecular Recognition:** Molecular recognition and self-assembly through interacting charged regions.

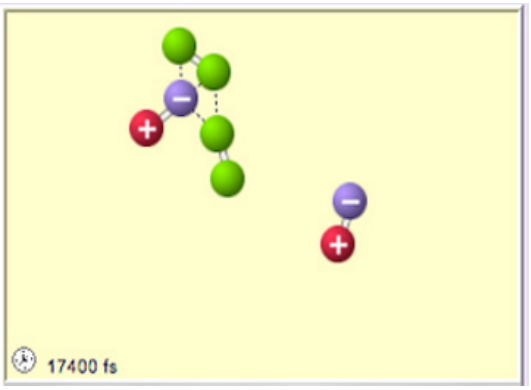
PHYSICS	CHEMISTRY	BIOLOGY
Atoms and Molecules		
A1. Atomic Structure: The atomic structure of atoms and molecules in terms of protons, neutrons, electrons, and quantized electron energy levels, and Periodic Table.	**A3. Chemical Bonds:** The physical nature of covalent bonds and the resulting dipoles; the disassociation of diatomic molecules and their energy.	**A5. Macromolecules:** Biological molecules, monomers, and polymers with their higher-order structures. The "Tree of Life".
A2. Electron Orbitals: Bound states of quantum systems; the relation between localization and energy levels (hydrogen orbitals, delocalized electrons, and electrical conductivity).	**A4. Reaction Rates and Catalysis:** The making and breaking of bonds in models that conserve energy. (Elementary reaction pathways and the role of bond energies, activation energy, and catalysts).	**A6. DNA and Proteins:** Formation of polypeptides, sequences of DNA and the resulting protein chains folding in water or lipids. Mutations.
Light		
L1. Photons: Photons and their interactions with atoms, energy levels and their effect on the spectra of absorbed light.	**L3. Photochemistry:** The energy-conserving interaction of photons with molecular bonds.	**L5. Photosynthesis and Vision:** The interaction at the atomic level of light with pigments such as chlorophyll and rhodopsin.
L2. Black Body Radiation: Links between thermal and photon energy. Black body radiation as the release of photons from thermally excited states.	**L4. Spectroscopy:** The relationship between excited states and spectral lines, with a special emphasis on bonds and IR spectra and applications.	**L6. Fluorescence:** The relationship of energy levels to the colors of fluorescence.



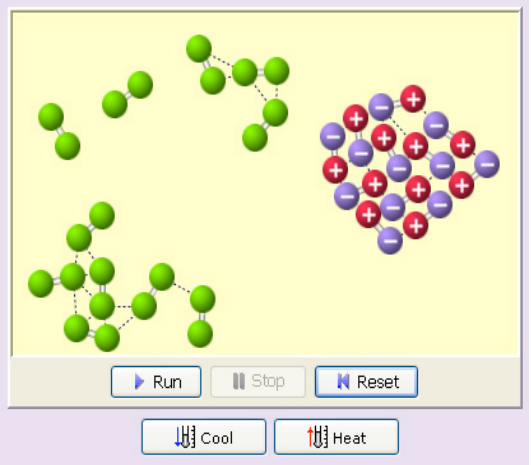
Progressions of Introductory Science Atomic- and Nano-Scale Concepts. This diagram shows the major interdependencies of the proposed topics described above. The columns correspond to physics, chemistry, and biology, the rows to the four strands, and the arrows connect activities that provide critical content to activities. It reveals that the light strand (at the bottom) could be optional, but the other three strands –in Motion and Energy, Charge and Atoms and Molecules--are quite interdependent. Most of the biology activities on the right are particularly dependent on several prior activities. The diagram also reveals some unexpected dependencies, such as the critical role of dipoles in the physics strand and the non-bonding forces (Forces between Atoms) in the chemistry strand. It also underscores how much more biology content can be treated given a foundation in physics and chemistry

SAMPLE UNIT: WEAK ATTRACTIONS

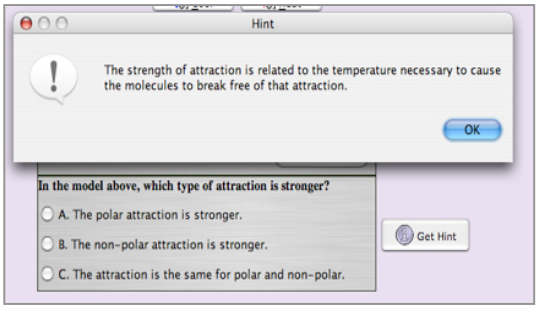
URL: http://molo.concord.org/database/activities/227.html



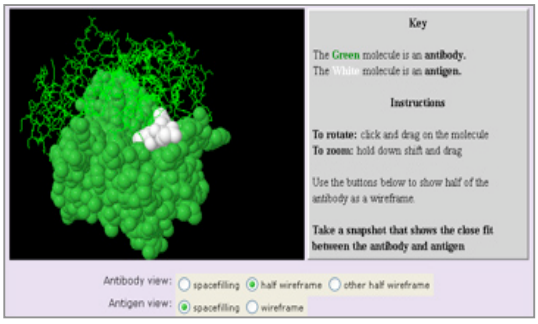
1. The unit begins with students exploring a mixture of polar (red and purple) and non-polar (green) molecules. They select different molecules as "probes", bringing them close to other molecules, thus making and breaking van der Waals (VDW) attractions depending on proximity. They discover that both polar and non-polar molecules are attracted to each another.



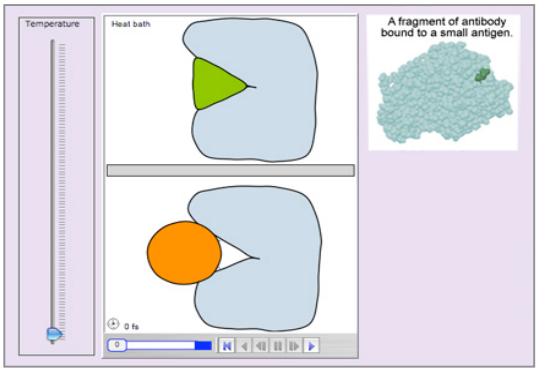
2. Students work with two liquid compounds, one polar and the other non-polar. They use heat to test the strength of the intermolecular attractions, and discover that in polar compounds the attractive forces are stronger, requiring higher temperatures to vaporize the polar substance.



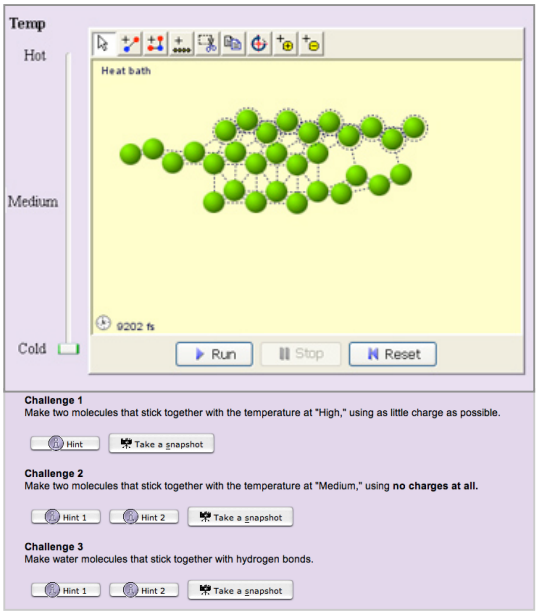
3. Students can choose to view hints as needed to help guide their inquiry.



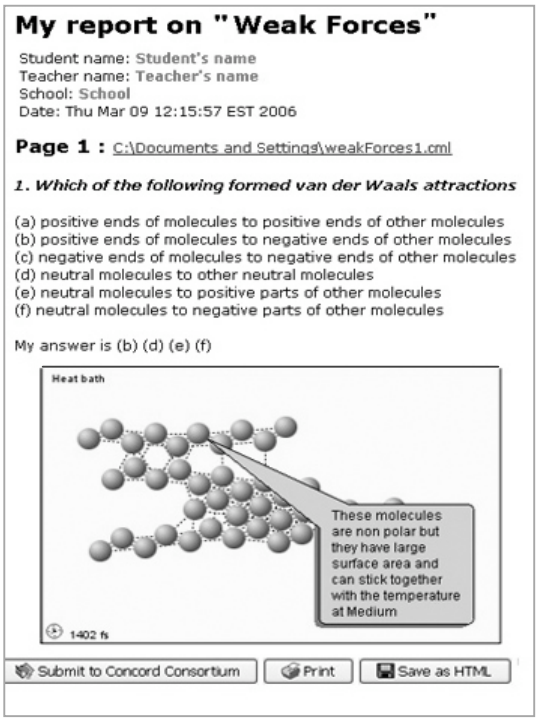
4. To bring relevance, students explore attractions between two molecules, an antibody (green) and its specific antigen (white). They discuss with each other how the antibody can attract and stick to its specific antigen. Using an interactive 3D molecular viewer, students uncover the inner structure of the antigen-antibody complex.



5. In this dynamic model two identical antibodies interact with two different antigens, one that fits an active site (green) and one that does not (brown). Students discover that the attractive forces between the molecules increase with an increase in the area of complementarity. Using heat, they can assess the strength of the attraction.



6. Students undertake a set of challenges to test their comprehension. One of the challenges calls for students to create a set of non-polar molecules that can still stick together under moderate temperatures. Students design molecules with different charge distributions, experiment with changes in temperature and explain their results. Students should determine that such compounds will be composed of molecules with large interacting surfaces, allowing VDW attractive forces to be significant enough to resist disruption by heat.



7. Student answers to embedded multiple choice questions and essay questions, as well as their annotated snapshots, are automatically collected in a Final Report and recorded in a report that can be saved on the server as an HTML file or printed. Students use callouts in the snapshots to point to specific areas of the model to describe their observations. Collections of annotated snapshots representing different stages of the modeling activity can be saved. Teachers can use Final Reports to assess student understanding.

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