Molecular Visualization in Science Education

Report from the
MOLECULAR VISUALIZATION IN SCIENCE EDUCATION WORKSHOP
NCSA Access Center, Arlington, VA
January 12-14, 2001

Sponsored by the National Science Foundation
NSF Award REC-0090523

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Preface

There is usually a long gap between technological innovation and its application in education. Sometimes this is because educators and teachers do not see its relevance and sometimes because of the capital and recurrent costs of using the innovation.

However, from the early days of computing, it was recognised that the innovation would make a major impact in education and some of those who had the foresight and perseverance were amongst the participants of this workshop and must feel vindicated.

Some of the greatest advances in science recently are in the area of molecular biology, which enfolds many of the branches of the great disciplines of biology and chemistry and these have been made possible by the use of computation, particularly by the way we can now look at molecular structure.

In the early days these techniques needed computers at the very forefront in terms of size and cost. Then 15 or so years ago microcomputers became available, which allowed for desktop structural computations in research and thence led to programs on molecular modelling that could be simplified for university and school biology and chemistry curricula.

This is of great significance, for chemical education demands so much from students. It requires them to understand abstract theories, (sometimes two to explain one phenomenon!), to have mathematical skills, to have experimental skills, to be able to communicate orally and in writing and to visualise in three dimensions given information in two dimensions. And that is just the start.

Visualisation of even simple molecules or crystal structures in three dimensions, even the position of a functional group in a small organic molecule is found by many students to impose an almost insuperable hurdle to their understanding, a problem borne out by research over many years. They need help to obtain a concrete model. Just like the researchers in molecular recognition working on similar if more complex systems.

This workshop and the 2001 Gordon Research Conference on Science Education and Visualization are special for two reasons. First, they bring educators together with scientists and cognitive psychologists, allowing each group to break out of its box in which the members talk only to one another, and the three groups can then learn from each other. Secondly these are timely events, as we are literally on the threshold of being able to realise the dreams of those pioneers as more and more investment is made by universities, colleges and schools across the world in hardware and software for instruction.

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Background and Overview

This document reports on a workshop that was held to consider how we can help students visualize and comprehend the molecular level of matter. The workshop, which was funded by the National Science Foundation, was held at the National Center for Supercomputing Applications ACCESS Center in Arlington, Virginia on January 12-14, 2001. Scientists, cognitive psychologists, and science educators came together at this workshop to examine how scientists use representations of chemical structure, mechanics, and dynamics to communicate ideas and how students can best learn from them. See http://pro3.chem.pitt.edu/workshop/ for more details.

The workshop was the first part of a National Science Foundation-funded effort to support collaboration among diverse research communities in order to define the role of and encourage research into the use of molecular visualization in science education. The second part of this effort is support of the 2001 Gordon Research Conference on Science Education and Visualization and the third part is the awarding of mini-grants to support new collaborations related to the study of visualization in science education.

The goals of the workshop were to:

- identify characteristics of molecular representations and visualizations that enhance learning.
- identify the types of interactions with molecular visualizations that best help students learn about molecular structure and dynamics and explore new technologies that show promise for this application.
- identify the roles of molecular modeling in college chemistry curricula.
- recommend fruitful directions for research on molecular visualization in science education.

Prior to the workshop participants commented on these goals and posed questions for discussion. At the workshop Andrew Johnson, Nate Lewis, Jeffrey Madura, Barbara Tversky, and David Uttal gave opening perspectives and a variety of projects incorporating molecular visualization were demonstrated. Participants broke into four working groups to address the first three goals and all groups prepared recommendations on research directions. This document reports on the group discussions and recommendations. Although it focuses on molecular visualization it is intended to stimulate thinking on how the three disciplines of science, cognition, and education can be joined to study and improve visualization in all fields of science education.

We would like to express our appreciation to Mindy Correll at the University of Northern Colorado Mathematics and Science Teaching Center for assistance in conference planning and to Tom Coffin and the rest of the staff of the National Supercomputing Center ACCESS Center for providing a facility ideally suited to the interactions, demonstrations, and connectivity we required. We also want to acknowledge Nora Sabelli and Lee Zia of the National Science Foundation for their guiding vision and support, the workshop advisory board for contributing direction and literature, and the workshop participants for their enthusiastic participation and generous sharing of their time and ideas.

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Workshop Organizers

A Context for Molecular Visualization in Education

Learning Science

For professional scientists, learning science is a life-long enterprise. The occasions of learning are varied, encompassing spontaneous reflection, reading, course work, interactions with colleagues, the acquisition of laboratory and mathematical techniques, and research itself, for it is useful to think of research as an activity in which the individual rediscovery that typifies most learning is transmuted into discovery that is new to others. When we ask how to improve science learning, then, we are asking about some of the most extraordinary and complex developmental changes that occur in the human mind and brain.

The workshop reported here was an attempt to further the growing and critical interaction between the sciences of learning and the learning of science. The workshop focused on the changes in science education sparked by the rise of computational chemistry and by the widespread availability of computer-based visualization tools. The dual premises of the workshop were, first, that molecular visualization in chemistry education is an important context for exploring the educational implications of recent advances in the cognitive and learning sciences, and, second, that questions about the optimal usage of molecular visualization for both education and research can provide an important stimulus for new research on cognition and instruction.

Why Chemistry?

Because the understanding of spatial structures and processes is central to the discipline, chemistry is an ideal site for exploring questions about the use of computer-based visualization and animation that are arising throughout science education. Conclusions about the sound design of graphical displays and animations should have wide applicability in other sciences.

P. W. Atkins (1987) once noted with approval that the subtitle of a widely used chemistry text was *The Central Science*, a phrase that captures chemistry's role in linking physics and biology, and hence its crucial conceptual position in science education as a whole. Enhancements to chemistry education can have powerful positive effects on the rest of the science curriculum. (Note that the cognitive scientists who participated in the workshop are practitioners of another central science, which links biology and psychology.)

Goals for Science Learning

Science instruction must address the notably complex nature of science learning. Instructors in a given instructional context can select from a range of goals, which may or may not be achieved by students. As graphical displays and visualization tools are increasingly introduced into science education, the possibility of new learning goals arises. It is therefore important to reflect on current learning goals and how new tools may affect what and how much we expect students to learn.

Recent national studies (AAAS, 1994; NRC, 1996; Advisory Committee, 1996) have converged on the recommendation that multi-leveled science learning goals be pursued in parallel throughout the K-16 curriculum. The authors argue that the facts and procedures students are learning should always be put to work in concurrent learning activities that involve the active application of concepts and scientific inquiry. A reconsideration of the goals of science education and the results of learning research both support this approach to instruction.

When science is taught mainly as a collection of facts that serve as prerequisite knowledge to later learning, many students finish their scientific education with misconceptions of the nature of scientific research and little ability to think critically about scientific issues. They may become citizens who are neither inclined nor equipped to think through the intrinsically scientific issues that permeate the workplace and the public sphere today. Introducing all students to a deeper appreciation of scientific theories and inquiry should be a central goal of science education. Those students who wish to go on to advanced levels often struggle to make the transition from memory-based performance to the active use of scientific concepts in novel, open-ended situations. Educating more individuals, who are more analytical and creative, should be a central goal of science education.

There is solid evidence that infusing the entire K-16 curriculum with learning activities that involve inquiry and active concept mastery can contribute to the goals of a more scientifically sophisticated citizenry and a stronger research community. Contemporary cognitive and educational research has shown that conceptual, inquiry-oriented knowledge is more persistent, provides better support for future learning, and transfers more readily to novel situations than list-like factual knowledge or rote problem-solving procedures (NRC, 2000). Educators have begun to articulate key scientific concepts and inquiry experiences that are appropriate for different grade levels (NRC, 1996), and recent educational research and development have demonstrated learning activities, instructional methods, and materials that can support the desired learning outcomes throughout the K-16 curriculum (NRC, 2000; AAAS, 1994).

The learning goals in the new science standards can serve as a framework for the development and assessment of new educational materials and instructional approaches that incorporate technology-intensive visualization. Visual media and software should be designed with clear learning goals in mind, and their refinement and revision should be guided by the careful assessment of whether students are attaining the goals.

It is particularly important that K-12 teachers have a firm grasp of molecular concepts. Visualization tools such as molecular modeling and animation can be used in teacher preparation to give teachers an accurate and rich picture of the dynamic nature of molecules and molecular interactions – which often they will not use in the same way with students – but at least they have the right picture on which to build their instruction.

Vision and Visual Thinking

From an evolutionary perspective, vision is an adaptation that allows organisms to extract information about the macroscopic three-dimensional physical world from light reflected by physical surfaces. Vision in primates involves an extraordinarily complex computational system, including numerous specialized regions of the brain (Kosslyn, 1994). The potential of visualization for education stems in part from the sheer power of the information-processing resources available in the visual system and in part from subsystems that are specialized for different tasks, including

- Representing the shapes and relative spatial positions of objects in the immediate environment over time.
- Memory for visual patterns and visual concepts. The staggering capacity of visual memory is suggested by our ability to recognize many thousands of objects. Its powers of

generalization and abstraction are suggested by our ability to assign a wide range of objects, varying in size, orientation, shape, coloration, and texture, to a category such as "dog." Visual memory vastly expands our ability to understand what we see and to take appropriate action (an informative empirical and theoretical exploration appears in Chase & Simon, 1973 and Simon & Chase, 1973).

- Visual imagination. The visual system can synthesize representations from information in thought and memory rather than from retinal input, allowing us to predict transformations in the physical world and to plan our interventions in it (see Shepard & Cooper, 1982 for a series of classic scientific studies of visual imagery).

The visual system is thus a powerful educational resource. If science content can be cast in visual form, the learner can benefit from the system's formidable powers of spatial representation and transformation, memory, and concept formation. Note, however, that experience with a particular class of visualizations may be necessary for comprehension. Spatial patterns and transformations that are specific to the visualizations take time to learn.

The visual system is also artfully designed to conceal its limitations from consciousness. We experience a uniform visual field in spite of the fact that full pattern processing is only available in a small region a few degrees in diameter in the current direction of gaze. Even within this region a limited-capacity neural resource seems to be required to bind separate features into coherent object representations (e.g. Treisman, 1985). The neural resources for tracking the identities and spatial locations of particular objects also appear to be limited in capacity (Trick and Pylyshyn, 1994). In educational settings, the visual system should not be treated as if it has unlimited capacity. Visual displays can be too complex to process, particularly for the inexperienced. Designers who have learned the patterns and practiced the transformations represented in such displays may be unaware of the challenges they pose to novices.

Imaging Technology

The strength of the human desire to extend the powers of vision beyond immediate physical circumstances is suggested by the fact that imaging technologies are among the earliest and most widespread manifestations of culture (Tomasello, 2000). It is of interest in the present context to note the prominent role played by chemistry in the development of imaging technologies, such as painting, printing, photography, and electronic imaging. The continuous historical development of these technologies has brought us to the threshold of virtual reality (which, of course, promises to involve the non-visual senses, as well). We have arrived at the moment in human history when any idea we have about synthesizing a visual experience can be realized. In education, we can for the first time envision the potential of visualization without regard to technical limitations.

Visualization

The term *visualization* is used traditionally to refer to activities of visual imagination and has been extended to apply to the creation of external images that extend our visual experience or imagination. Visualizations bridge gaps between ordinary vision, which is powerful but depends on the presence of the relevant parts of the actual world, and visual imagination, which functions without sensory input but is highly limited in capacity. Visualizations extend visual memory and thought by providing virtual worlds for vision to work on. A neurosurgeon, for example, can visualize a brain tumor by imagining its location or by inspecting magnetic resonance images of the patient's brain. The MRI images augment the mental image of the surgeon, who can in turn transform his or her image to plan a surgical approach or to consider the possible need for further tests. External visualizations also serve valuable communication functions. The MRI images can help the neurosurgeon communicate his or her understanding of the tumor to the patient, who ideally acquires an internal image that resembles the surgeon's.

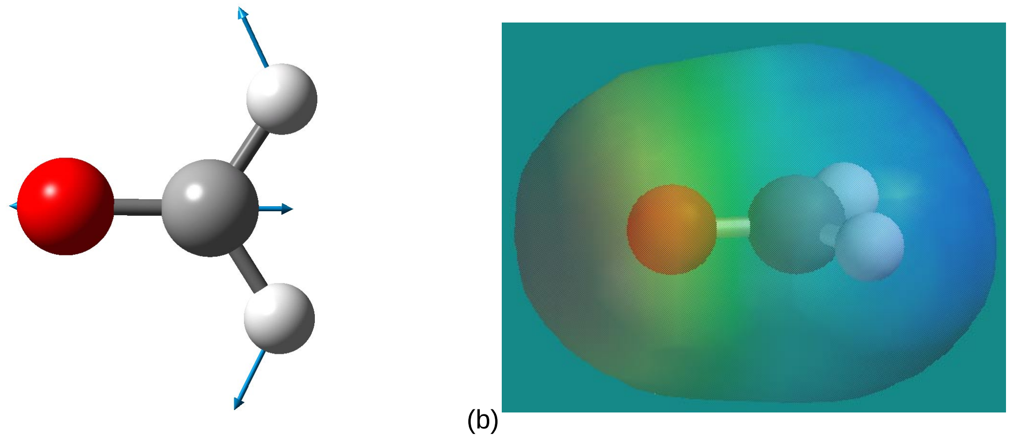
Thinking clearly about the role of visualization hinges on understanding that the immediate significance, or meaning, of an internal or external visual image depends critically on an intended interpretation. That is, the meanings of images involve relations to other things and ideas. These relations are symbolic in the sense that they are matters of convention that involve some degree of arbitrariness. Some conventions exploit natural correspondences that facilitate image understanding. Perspective rendering, for example, exploits a natural projective correspondence between three-dimensional and two-dimensional space. The time lines and number lines used in graphs exploit cognitively natural correspondences between time or number and spatial extent. Nevertheless, the need for interpretation is never fully eliminated. In intellectual contexts particularly, the proper interpretation of an image is not fully encoded in its spatial structure.

Consider our hypothetical neurosurgical situation again. Magnetic resonance imaging maps numerical data representing tissue density onto two-dimensional brightness or color values that are displayed for human visual perception. Interpreting one kind of MRI image requires knowing that it represents a particular cross section of the brain in a particular left-right and top-bottom orientation, that particular areas of the two-dimensional image represent functionally-significant three-dimensional structures in the brain, and that brightness values are correlated with particular types of tissue and states of health. Although the neurosurgeon can "see" the diagnosis at a glance, the image is initially meaningless to the patient, who lacks the surgeon's knowledge of neuroanatomy, MRI imaging conventions, and typical spatial patterns that show up on the images. The surgeon's conference with the patient becomes a mini-course on neurology, MRI, and the network of conceptual relations that connect them.

Visualization in Science Learning

The above remarks suggest that the usefulness of a visualization to students depends on knowledge of concepts that the visualization is designed to represent. For example, a student cannot learn from space-filling models of molecules without at least rudimentary concepts of *atom, molecule, carbon, oxygen,* and so on. Students must also understand something about the mapping between the models and the concepts; for example, black or gray spheres represent carbon atoms, red spheres represent oxygen atoms, and white spheres represent hydrogen atoms (see Fig. 1a).

If students are to learn something new from a particular display, they must attend to relevant aspects of the display and appreciate how they illustrate new concepts. For example, the conceptual point of an electrostatic potential diagram (see Fig. 1b) is not that a molecule consists of connected atoms in a cloud of electrons, but that the distribution of electrons across different atoms may be of conceptual importance. The typical learning situation utilizing visualizations, then, involves a process of bootstrapping in which students are simultaneously learning about and from the displays, that is, learning both new concepts and how those concepts are visually represented in images that are intended to facilitate learning the concepts. Fluency with the visual conventions employed in a particular type of visualization develops with time, ultimately leading to the expert’s fluent perception of the conceptual relationships that are encoded in the displays.



(a) (b)

Figure 1. Two representations of the same molecule designed to convey different information. In (a) a molecular structure is shown as a ball-and-stick model. The red sphere represents an oxygen atom, gray carbon, and white hydrogen. The arrows represent relative degrees and directions of motion as the molecule flexes and vibrates. (b) The molecule is viewed from a different angle to better show the electron distribution above and below the plane formed by the atoms. The "cloud" surrounding the structure represents the molecular surface formed by the electrons that circulate through the molecule. The colors in the cloud show how the electrical charge of the electrons is distributed across the surface, with its highest density around the oxygen atom. (Image produced by Jeffry Madura using Spartan from Wavefunction, Inc.)

Properties of Molecular Visualizations

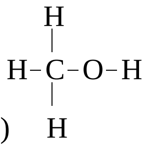
Each area of human knowledge offers different possibilities for visualization. In more concrete cases visual displays represent visible, physical spaces. The everyday macroscopic physical world can be represented, for example, by static 2-D visual displays that partially simulate visual experience. Examples are perspective drawing, photographs, cartoons, and architectural plans and elevations. These concrete displays make use of various kinds of simplification to focus the viewer's attention and clarify important elements or relationships. Photographs stop motion and are carefully framed and focused. Cartoons emphasize contour and exaggerate key features. Floor plans display only ground-plane spatial relationships. In more abstract cases effective visual representations have been invented for domains that are not intrinsically spatial. Flow charts, evolutionary trees, ecological networks, and graphs of economic variables over time are examples. Abstract displays take advantage of natural mappings from non-visual conceptual/perceptual domains onto visual: Higher-pitched notes are higher on the musical staff; numbers and times are laid out on vertical or horizontal lines in 2D displays; temperatures are mapped onto "cool" and "warm" colors; the tail of an arrow represents an earlier time than its head (see the arrows in Fig. 1a and the colors in Fig. 1b). The periodic table is a superb example of how the horizontal and vertical dimensions can be combined in a 2D tabular display to organize conceptual information.

Molecular visualizations are a complex hybrid of concrete spatial depiction and abstract visual encoding. They represent physical objects and therefore depict spatial relationships in the world (rather than using space in the display to represent something else in the world, such as the price of a stock). On the other hand they employ numerous symbolic graphical conventions to highlight and locate in space theoretically important aspects of molecules; for example, by color-coding the elements, representing molecular bonds as thin material rods or by representing electron distributions as volume-enclosing surfaces, as in Fig. 1b.

Many chemists believe that the real power of computers and visualization in chemistry is their use in helping students understand the dynamics involved in chemistry; for example, that proteins are flexible and not rigid entities, the mechanism by which ions get through biological channels, how heating a molecule increases its reactivity, and the origin of phase transitions. Visualizations are important in this context in that the effect of subtle interactions between molecules, which are complex and difficult to describe simply, can be grasped in a glance.

Potential Implications of Molecular Visualization

Visualization in chemistry is part of the general multimedia explosion in science education, which is characterized by the design of custom visualizations to illustrate particular structures or concepts. The better illustrations are informed by general principles of good visual representation and graphic design, but the linkage between scientific concepts and visual representation is often not deeply principled or algorithmic. Textbooks in physiology or geology, for example, contain hundreds of illustrations that opportunistically employ a huge range of graphical conventions to illustrate numerous structures, processes, and models that are related to each other but not strongly integrated theoretically. In chemistry, however, a unified theory is used to make quantitative spatial predictions, which allows highly generalized rules to link theoretical concepts to visual displays. Expanded structural formulas that show the connectivity within a molecule by lines connecting the elemental symbols of the atoms, are an example of a type of productive visualization, in which a set of diagrammatic rules produces qualitatively informative diagrams of an unlimited range of molecules (Fig. 2). In contemporary chemistry the possibilities have been expanded by using computer-based numerical representations and graphical rendering algorithms in molecular modeling programs to produce spatially accurate graphical displays of molecular structure and dynamics.



$$\begin{array}{cccccc} & & \mathrm{H} & & & \\ & & | & & & \\ & \mathrm{H}- & \mathrm{C} & -\mathrm{O}- & \mathrm{H} & \\ & & | & & & \\ & & \mathrm{H} & & & \end{array}$$

(a) (b) CH_3OH

Figure 2. The expanded structural formula of methanol (a) conveys more information about the molecule than the condensed structural formula (b).

<u>The promise for students</u>

Because basic 3D spatial relationships in molecules have systematic and profound causal significance, chemistry is an extraordinarily fertile field for visual learning. To learn chemistry is in part to learn how chemical concepts play out in space and how spatial relationships signal theoretical meanings. It is in part to learn how to use diagrams and displays to aid understanding. Typically students enter chemistry courses with persistent misconceptions about the particulate nature of matter (Gabel, Samuel, & Hunn, 1987). Visualization tools provide a means of helping students improve their conceptions. Teaching chemistry involves helping students grasp the spatial dimensions of chemical theory, as they simultaneously learn about and learn from the visualizations that are employed in the field. A student's struggle to master the meaning of a particular display nearly always has the potential to transfer to other displays and problems, because displays are based on general principles and are used consistently in beginning and advanced work. Since visualization is intrinsic to research in chemistry, learning to work with visualizations can be integrated with active, problem-based, or inquiry-oriented learning activities that mirror the research experience.

The potential for educational technology

The productive, algorithmic nature of computer-based molecular visualization opens up exciting possibilities for educational technology. The possibilities, discussed further below, range from intelligent skill-building tutors to virtual reality molecular worlds to student research projects using molecular databases.

Learning with Molecular Visualization

Its highly systematic and conceptual nature make molecular visualization an ideal arena for visual learning. From the standpoint of theories of vision, cognition, and learning, however, it also poses highly significant challenges to the learner. The difficulties that students might face in understanding and using molecular visualizations can tentatively be divided into four areas:

Visual subtlety

Basic spatial relationships in molecular displays, even when they are faithfully rendered, challenge human visual capacities for at least the following reasons:

- Angular relationships that are not 90 degrees and that therefore can not be aligned with orthogonal 3D coordinates are significant. Orthogonal relationships, particularly when aligned with the horizontal and vertical, are relatively easy to perceive. Non-right angles are relatively difficult to perceive, particularly when they are not embedded in a picture plane (a plane orthogonal to the line of sight). The relative difficulty is amplified in 2D perspective views, which lack some depth cues (e.g. stereopsis and head-motion-induced parallax), but is still present for actual 3D models or virtual reality displays.

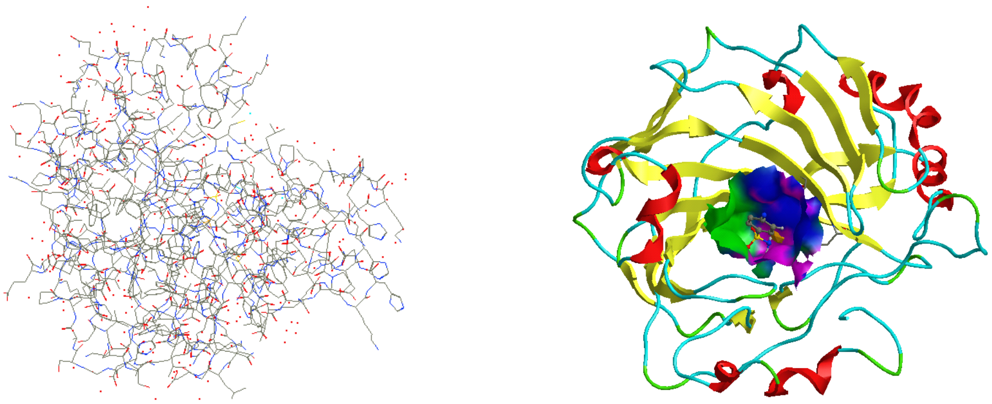
- The values of distances and angles are sometimes significant. Precise metric values are generally not directly perceivable, and relative values can be difficult to perceive, particularly when they lie in different 3D planes. The difficulty is exacerbated by 2D perspective representation.

- Spatial relationships among three or more parts of a molecule are often significant. Limitations on visual attention make it difficult to grasp the arrangement of multiple objects in space. Tracking multiple objects in motion is very difficult.

- Relationships that involve symmetry, reflection, or rotation are frequently significant in molecular visualizations. Although symmetry about a vertical axis in a picture plane can be readily perceived in two dimensions, symmetries in three dimensions are more difficult to perceive. The "handedness" of objects is not directly perceived. It is therefore difficult to distinguish between two objects that differ only by reflection. The mental comparisons or rotations involved in appreciating 3D correspondences, or the details of 3D shape, are effortful and error-prone.

Complexity

The amount and depth of the information that potentially can be encoded in visual displays makes molecular visualization exceptionally complex. The complexity has been managed through the design of different types of displays to represent information at different spatial scales or to highlight particular theoretical analyses. Students are confronted with many different types of displays, including structural formulas, organic line structures, Lewis structures, ball-and-stick models, space-filling models, electron-density models, protein ribbon models, and other computer-generated graphics and animations (Fig. 3). On the one hand, students benefit from the tuning of the visual elements of each type of display to its conceptual content. On the other hand, learning to understand each type of display and the interrelations among them is a formidable learning task.



(a) (b)

Figure 3. Two modes of representing protein molecules. In (a) only the bonds between atoms are depicted (by lines) and the surrounding water molecules by the red dots. This representation facilitates the study of how different regions of the protein interact with water. In the more abstract structure in (b) the red ribbons represent alpha helix regions of a protein and the yellow ribbons beta sheet (planar) regions. This representation shows at a glance how the long chain of atoms making up the "backbone" of the protein is arranged. Each representation allows the viewer to focus on important properties by leaving out less relevant parts of the structure.

Abstractness and conceptual depth

The earliest stages of learning are complicated by the need to master the relatively abstract graphic conventions involved in any depiction of molecules, which we do not see at the molecular scale under normal conditions, and which therefore do not have natural visual appearances. Ball-and-stick models, for example, mix spatial realism and graphic convention in a way that is beautifully adjusted to their purpose but potentially quite opaque to beginners. Balls and sticks are symbols that stand for things that have few of the properties of the symbols themselves. Students must learn to "read" these symbols, much as they learn that a double blue line on a map represents an interstate highway and that a small white square on the line represents an exit.

Throughout learning, students must confront the conceptual depth of molecular visualizations, which depict physical objects, but which cannot be understood, sensibly manipulated, or created without understanding the concepts that they are linked with. The theory of chemical bonds, for example, determines much of what we see in a molecular visualization, but the display encodes consequences of the theory, not the theory itself.

For expert chemists the cognitive links between theory and appearance are so fluent that they "see" the theory in the display. For novices some of these links may not exist and others may require effortful recall. Merely looking at the visualizations does not instill the relevant concepts. Experts amplify their well-established knowledge by carefully selecting visualizations to support memory and thought or confirm predictions. For the novice learners this feedback, or bootstrapping, relationship between a visualization and underlying concepts is much more delicate because of the relatively fragile state of their conceptual knowledge and experience with visualizations. In order for a display to enhance their use of a concept, they must already have some grasp of the concept and how it maps onto the display. In order to learn more about a concept from the display they must already know and be able to remember something about the concept. If the scaffolding knowledge fails, the visualization becomes meaningless, a sentence in a foreign language. If it succeeds, the visualization may contribute significantly to both momentary understanding and long-term conceptual mastery.

The visual subtlety, complexity, and conceptual depth of molecular visualization pose significant challenges to learners and teachers, and they raise important research and design issues for curriculum developers and educational researchers. Some of the issues are outlined below.

Individual and Group Differences in Learning

The novice learner, invoked in the above discussion, is a statistical mode that stands for a range of individual differences among students in entry-level spatial cognition and reasoning. It should not be assumed that any change in the use of molecular visualization in instruction will increase the range of students who master chemistry. It would be relatively easy, in fact, to design a rapidly-paced, visualization-intensive curriculum that would disadvantage students with weak entering skills in visual cognition.

Individual differences sometimes reflect group differences that are of current social importance. For example, gender differences, favoring men, in understanding and imagining spatial transformations, such as rotation, are among the largest and most consistent that have been reported in the general psychological literature. If this difference plays a role in college chemistry performance, chemistry instruction could play either a positive or negative role in women's entry to scientific careers, depending on whether students are given adequate opportunity to learn visualization skills. Cultural differences may also influence how students use and learn from visualizations.

Molecular Visualization in the Curriculum

The centrality of molecular visualization in the field of chemistry suggests that its role should be considered in relation to the full range of goals for science education that have been articulated in recent national reports (Advisory Committee, 1996; AAS, 1993; NRC, 1996). It should be noted that the points discussed at the workshop and presented here are motivated mainly by general theories of learning and instruction and by current work in educational technology. They will have to be shaped further by commentary and experience from the chemistry education community. No attempt is made here to assess the degree to which the suggestions made have been implemented.

Factual and Visual Fluency

High school and college science instruction has traditionally been over-balanced toward delivering relatively inert facts to students and testing them for rote retention. Facts should be acquired in environments that require their understanding and meaningful application. It is worth noting, however, some of the factors that affect the learning of facts in visualization-rich contexts.

Practice: Amount, timing, and feedback

As noted above chemistry is rich in nomenclature, structures, and multiple visualization types. Extensive practice is required to achieve any degree of fluency in such a complex domain. Software-based visualization can enhance the amount and quality of practice in several ways. The production of examples and problems can be automated (or semi-automated), increasing the number of exposures in a course, or achieving the same amount of exposure at the cost of less laboratory, problem-solving, or teacher time. Software-based tutors can generate immediate feedback and sequence exercises contingent on student performance. Because brief (10-30 minutes) practice sessions held three times per week or more appear to be effective during the first few years of complex skill acquisition, brief, relatively low-level, practice sessions with molecular visualizations should have a measurable pay-off for higher-level learning activities. The value of frequent practice can be enhanced through the immediate feedback provided by the use of web delivery and by several strategies such as those that follow.

Annotation

Verbal descriptions of visualizations are essential for pointing out their significant features and building relevant causal concepts. Descriptions are frequently unclear to students, however, because they are not sure how the words map onto the picture. In the classroom such misunderstandings are often cleared up by redundancy in the lecturer's presentation or by student-teacher interaction. The chances of confusion are much greater in computer-based presentation. Confusion can be reduced by providing students with a simple way to post questions or comments on material and by annotating the visualization itself. An advantage of computer-based over print presentation is that the density of annotation can be increased through step-wise animation of labels, arrows, color codes, and so on. The student can be given the power to step through and replay the stages.

Dimensional focus

Given the challenges that the structural subtleties of molecules present to human visual perception and cognition, it is unlikely that enough attention is currently being paid to helping students overcome them. The challenges could be specifically addressed in software-based tutorials. Properties such as dihedral angles, polyhedral structure, chirality, functional groups, or the dynamics of molecular conformations can be carefully explored through color-coding, rotation, or piecewise highlighting or animation. Using the simplest possible display that contains the target information is a useful strategy that is sometimes not followed in computer-generated presentations. Richer displays often contain irrelevant information that can distract or mislead the learner. Traditional molecular line drawings have much to recommend themselves in this regard. The ability easily to add or subtract elements of displays in molecular modeling programs is a very useful recent development.

Comparative presentation

The complexity of molecules and their representations can be addressed in part by presenting students with side-by-side comparisons of related displays. Comparisons as simple as frequently labeling visualizations with their chemical names or displaying expanded structural formulas next to their ball-and-stick or space-filling models are potentially of great value. The availability of display options in molecular modeling programs is an example of offering adventurous students the opportunity to explore a range of such comparisons. It can also be exploited by tutorial developers to support students' exploration. The simple idea of using visual comparison to clarify concepts is indefinitely extendable. Any visualization can potentially be clarified by comparing it to another that is similar but differs on a critical dimension. Guided visual comparison appears to be a very widely-employed strategy in both traditional and computer-based chemistry instruction. However, computer-generated visualization should allow many more, high-quality comparisons to be presented to students.

Animation

Animation can add considerable learning potential to computer-generated visualization. We might distinguish roughly between two uses of animation. First, animation can be used to clarify information that is essentially static. For example, by rotating a computer-generated molecular model, one can get a better appreciation of its 3D structure; by systematically assembling and taking apart the visualization of a crystal, one can clarify structural relationships. Second, animation can be used to visualize the dynamics of individual molecules or molecular interactions. There is much educational potential in both these uses, but the second seems clearly the most important, since it extends molecular visualization to the processes that are at the heart of chemistry. Bringing numerically accurate dynamic simulations of complex processes into the classroom is a particularly exciting prospect.

It should be said, however, that we know very little about how to use animation effectively in instruction. The proper role of animation in chemistry education should be treated as an issue in cognitive, educational, and curricular research. As animation is brought increasingly into the curriculum, its effects on students should be carefully researched.

From the standpoint of the cognitive science of vision, a clear issue is that displays of molecules in motion are extraordinarily complex. There will be cases where most novices fail to see what is important in an animation. One corrective strategy is breaking a continuous transformation down into static snapshots, which are then annotated and compared. Giving the user the ability to step through and stop transformations, and to turn various kinds of annotation on and off, should also be important. An example might be a protein folding into a certain large scale shape. It can be easy to see that two shapes fit together. On the other hand it can be difficult to track the relative positions of four or five atoms in a protein molecule as they move through the simulated folding (Fig. 4).

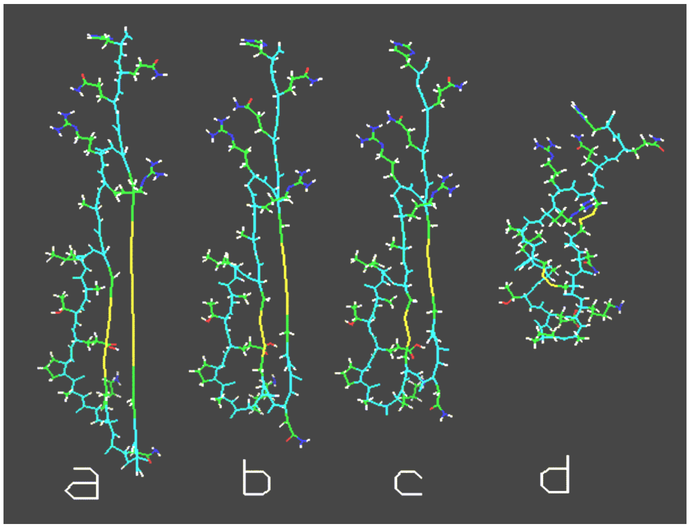


Figure 4. Four steps in the folding of a protein molecule. Showing the folding in separate steps makes it easier to comprehend the process by which the strand folds upon itself. (Image from *Molecular Universe*, by Richard Catlow and Clive Freeman; see www.moleculaaruniverse.com. Produced with WebLabViewerPro.)

Promoting Understanding through Interaction

If computer-based visualization were used extensively, following all of the recommendations above, and nothing else were done, it is likely that many students would not develop a very sophisticated understanding of chemistry. Students must do more than simply view well-prepared visualizations. One of the unfortunate drawbacks of current visualization technology is that when it is the sole means of learning about molecular structure and dynamics students simply observe what they once might have struggled to imagine or draw or build activities that may lead to deeper learning. A major goal for the use of computer-based visualization should be the provision for students to actively explore and use concepts.

Software interactivity

The most straightforward step toward increasing active student involvement in learning is to make visualizations interactive. There are a number of relatively simple forms of interactivity that are easy to apply. For example, students can be asked to answer multiple-choice questions about displays, to make predictions about displays, to point to critical parts of displays, or to manipulate a display (such as a computer-generated molecular model) in order to answer a question. Questions can be designed to tap different levels of conceptual understanding. With some additional development work item statistics can be collected on particular questions to confirm their difficulty level and the content of tutorials can be contingent on the student's answers. Most current visualization-based chemistry tutorials contain examples of good interactive questions but do not contain nearly enough interactive material to build conceptual understanding.

Interactivity that explores causality

A particular strength of computed molecular visualization is the ability to represent causal factors and processes more easily, more accurately and, in more detail than was traditionally possible. Tutorials can explore the consequences of factors such as precise spatial conformation, orbitals, and charge distributions. Emphasis should be placed on having students make theory-based predictions or answer theory-based questions about the consequences of these key causal factors. As students grapple repeatedly with why molecules are structured in certain ways and react in certain ways, relatively unconnected facts begin to be welded together into an explanatory conceptual network that is resistant to forgetting and that serves as an input to active problem solving.

Software-based classroom interaction

Although software interactivity helps to build conceptual understanding, the current state of the art is not sufficient to bring students to a decent mastery of chemical theory. Good human tutors bring certain things to their interactions with students that are currently difficult to embed in software. Human tutors, for example, can ask students questions about the theoretical significance of a representation and respond intelligently to their answers. Students' answers often reveal initial conceptions that are inconsistent with chemical theory or incomplete. The tutor can then pose a scaffolding question that asks the students to use what they know to think more deeply about the issue, or to consider another case. By actively using their concepts in this kind of tutorial setting, students rebuild and extend them. Artificial intelligence applied to this purpose may one day lead to effective computer-based tutoring.

In a moderate-size electronic classroom, one way of achieving concept-driven tutorial interaction is to have students work individually or in pairs with visualization or simulation software to answer conceptual questions posed by the instructor (Khan, 2001a, 2001b). The instructor polls one or more students/pairs for answers and justification and suggests further lines of exploration with the software to test theories or resolve disagreements. The interactions set up a Generate, Evaluate, Modify (GEM) cycle that progressively builds concepts from the student's initial conception. These approaches can be modified to meet the needs of large lecture classes (Mazur, 1997).

Another approach to achieving a high level of student interactivity is the use of palm computers with simulation and modeling programs in the classroom. At the University of North Carolina-Wilmington students in large general chemistry classrooms use HyperChem modeling software on hand-held computers with wireless Internet access to create, modify, and make measurements on molecular structures (Shotsberger and Vetter, 2001).

At the high end of technological development are novel learning environments that help students to visualize complex or invisible phenomena. For example, the haptic arm is a “mouse” that allows students to sense attractions and repulsions as they interact with three-dimensional molecular structures. Virtual reality tools such as the Immersadesk and the Narrative-based Immersive Constructionist/Collaborative Environments (NICE) developed at the University of Illinois at Chicago are used to create, enter, and study representations of fundamental scientific ideas in a three-dimensional virtual environment (Johnson, 2000). Figure 5 shows students collaborating on the exploration of a virtual world. The goal of this application is to strengthen student understanding by allowing them to form mental models of abstract concepts by experiencing and controlling multiple representations of the concepts.

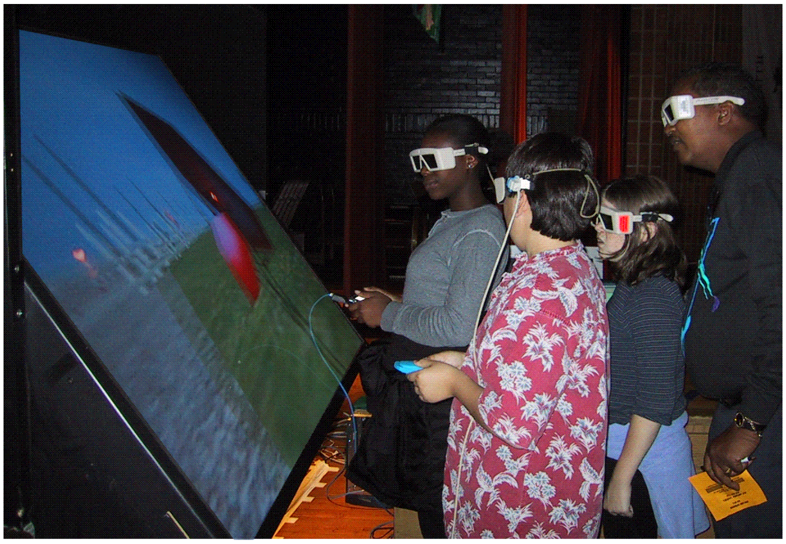


Figure 5. Sixth grade teacher Kevin Harris watches as three of his students explore a virtual world at Abraham Lincoln Elementary School in Oak Park, Illinois. One student drives the group through the space; another records the data they find using the Pocket PC; the third tracks their progress on a laptop computer. (Photograph courtesy of Andrew Johnson.)

Active Concept Mastery and Inquiry

If students are to be encouraged actively to explore and master concepts, at some point visualization and simulation software must become a tool that they, as well as their teachers, are putting to use. Individuals or groups of students can be assigned to prepare and present visualizations that they have created to solve a problem, verify a prediction, or illustrate a reaction. In such problem-based learning students become producers as well as consumers of visualizations and are forced to grapple with the concepts underlying their work. A higher education example of this kind of work comes from the University of Michigan, where groups of introductory students study and report on chemical synthesis problems over a period of weeks, defending their work to teachers and peers (Coppola, 2001). An example from the secondary school level is the *ChemDiscovery* curriculum, in which students construct their own learning pathways using highly interactive CD-ROM lessons (Jones, 1999). The teacher facilitates students' work as they design materials and compounds using extensive interactive databases.

Embedding the use of visualization tools in laboratory work that involves the collection and interpretation of empirical data is a final, crucial element in achieving an understanding of chemical theory and inquiry. Students must come to an understanding of how the highly abstract and symbolic visualizations that they have become familiar with are anchored in empirical observation. Visualization tools can also fundamentally change the way laboratory work is done–through an iterative process that uses the results of visualization tools to help design the next step in an experiment. One of the workshop organizers (Stillings) recently interviewed a professional scientist who reported that the most significant experience of his undergraduate career was trying to reconcile NMR data he had collected in a faculty mentor's laboratory with his theoretical ideas about what was supposed to have happened in his experiment. He became a scientist when his concepts (expressed as 3D line drawings and physical ball-and-stick models) bumped into the real world. A primary goal in developing the uses of molecular visualization in the curriculum should be to bring this kind of experience to greater numbers of students.

Summary of Recommendations

This section summarizes the main recommendations presented above and additional recommendations made by the four groups at the workshop. As stated previously, these recommendations are not intended to be either prescriptive or restrictive, but rather to stimulate dialog on molecular visualization among different research communities. Recommendations are divided into suggestions for fruitful research questions related to molecular visualization in science education and proposals for change in the chemistry curriculum. The central role of molecular visualization in chemistry and biology research today suggests that research into the scientific applications of visualization is as important as research into learning with visualizations.

Research on molecular visualization

Collaborations among chemists, biologists, cognitive scientists, and science educators may present new opportunities to study how students learn. Two types of approaches to research on the characteristics and usage of molecular visualizations were considered.
Macroscopic approach: large scale, long-term studies of the effectiveness of entire courses, including transfer.

- Microscopic approach: controlled studies comparing particular aspects of visualizations, such as three vs. two dimensions, the effectiveness of animation, and the degrees of schematization required for teaching specific concepts.

Characteristics of visualizations.

Analyze new visualizations produced by scientists: what drives the development of the visualizations? how are previous conventions used or changed? Where do new conventions come from?

- What are the effects of visualizations on intuitions, research questions, conceptions, and misconceptions?
- When are tactile interactions important?
- What are the effects of mixing different types of visualizations?
- How do individual differences such as gender, learning style, culture, etc., affect the ability to learn from visualizations?
- Is there a right-left brain shift in activation of visualization from experts to novices, comparable to that seen in music training?
- What principles of graphic design are important for the design of effective molecular visualizations?

Curriculum issues.

- What are the barriers to educators introducing molecular visualization into the classroom?
- What new student misconceptions might be introduced by visualization tools?
- How can networking, discussion groups, and other communication opportunities be used to support learning with visualizations?
- How can visualization best be used in combination with practical work in a hands-on laboratory setting? In groups of students?
- How do instructors use different visualization systems and representations? What do they use? For which topics? When?
- What pedagogical content knowledge is appropriate?
- Does working with visualizations require different kinds of problem-solving skills than are currently taught?
- How does knowing what a molecule looks like contribute to learning?
- How will the curriculum be restructured? (What must be given up?)
- How much guidance do we give students?
- How much visualization of a given type has to be present in a course for it to be effective?
- How can learning from visualizations best be assessed?

Interactions

Ideas for fruitful research questions included the following:

- How do student mental models of matter change as a function of interaction with molecular visualizations?
- How do student-generated representations change as a function of interaction with visualization systems?
- How do student-generated visualizations develop and change as students learn scientific concepts?
- Can we generate “thick” descriptions of students interacting with molecular visualizations to try to characterize the learning experience?
- What types of interactions are best for which types of situations or topics?
- How do students integrate different types of representations?
- Are different learning methods more appropriate for different situations? For example, is discovery learning preferable for qualitative notions, direct for quantitative?

Molecular visualization in the chemistry and biology curriculum

Molecular visualization provides new ways to talk about structure and dynamics and may thus be a stimulus for change in chemistry and biology courses. Workshop participants felt that such change must be undertaken with caution and expressed concerns about the appropriate use of molecular visualization in education. At present too many topics may be introduced to students at a time. We need to reduce the load on student working memory rather than add more. We also need to avoid introducing additional (and possibly confusing) variables along with the use of molecular visualization. For example, the hydrogen atoms in model kits are often too large relative to the other atoms, different model sets are used in lecture and lab, and some characteristics of representations may not be comprehensible to students. Introducing molecular visualization may also take time away from building problem-solving skills and may also be expensive.

The advantages of using molecular visualizations were seen as sufficient to make the effort of introducing them into the curriculum worthwhile. Molecular visualizations are believed to

- get students to think about chemistry in terms of molecules, models, and symbols.
- allow students to be more active learners.
- help students to understand models and symbolic representations.
- offer a chance to move toward change.

The interactive nature of visualizations encourages movement away from an instructor-centered paradigm of instruction in which students are passive learners toward a more student-centered approach in which students are active participants.

Develop approaches to visualization thqt are easy for students to use and interpret.

The abundance of different types of representations (chemical equations, mathematical formulas, graphs, animations, and different types of molecular representations) is a barrier to learning. Students can better cope with the variety of representations if the purpose of each type is discussed with students. It may be advisable to start with simpler structures, such as two-dimensional representations and move from them to more complex, three-dimensional ones.

Develop instructional methodologies that take advantage of the interactive nature of visualization.

Visualizing chemistry should be fun for students and hence motivating. Although visualization is not a “magic bullet” that can solve all the problems students have learning chemistry and biology, its use in classrooms provides many opportunities to raise the activity level of students. New technologies need to be explored to assess their potential as mechanisms for teaching visualization. For example, students in courses using a central computer server can collaborate and complete work that is tracked.

*Integrate visualization and modeling into curricular materials***.**

Not all topics can be taught with visualizations; the topics best taught this way need to be identified. Publishers play an important role in the kind of visualizations distributed and so need to be involved in the development of visualization curricula.

Support faculty who are introducing visualization.

Instructional materials for visualization need to be easy for instructors to learn and to use. In addition, faculty members need guidance and support when beginning to use molecular visualizations in teaching. Professional development and “in-service” opportunities are needed, as well as workshops on effective instructional strategies and on the research and dissemination of new ideas.

Develop a digital library for molecular visualization in science education.

The National Digital Library can be used to share information among chemistry instructors using visualizations. A common taxonomy of representations and terminology should be developed to help define the common ground.

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Resources

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Molecular Visualization Projects Contributed by Workshop Participants

Using Molecular Visualization to Demonstrate Principles of Protein Structure and conservation of Essential Function during Evolution.

A bioinformatics tool (the *Biology Workbench*) and a molecular visualization tool (*Protein Explorer*) are used in the teaching of molecular biology. The Workbench is used to align sequences of homologous proteins from widely different organisms and Protein Explorer is used to transform those alignments into three dimensional structural representations that illustrate functional conservation and principles of protein folding.
http://peptide.ncsa.uiuc.edu/educwb
Contact: Eric Jakobbson, jake@ncsa.uiuc.edu

Palm, Pocket, and Handheld Devices for Molecular Modeling

Handheld computers can now support sophisticated molecular modeling programs that are suitable for education and research. At the University of North Carolina-Wilmington students are issued handheld computers when they arrive for class. During class time they explore the properties of molecules and complete projects.
http://aa.uncwil.edu/numina/
Contact: Neil Ostlund, ostlund@hyper.com

Beneath the Surface of the Chemical Article

Beginning in 1996, a number of term-long projects were interwoven with the Structured Study Group program, in which first-year chemistry students earn honors credit. In one project, all of the students contribute to the construction of a written and HTML literature-driven resource on which their final examination is based. Ultimately, the multimedia text is fully owned by the students in the course, and they must seek out each other's expertise in order to examine their understanding.
http://www.umich.edu/~chemh215
Contact: Brian Coppola, bcoppola@umich.edu

ChemSense

ChemSense is a software environment that provides students with a variety of representational tools and resources that they can use to express their understanding of chemical phenomena. These tools allow students to create different types of representations and use them in a community of learners to make predictions and explain the results of their laboratory investigations. These representations are both student-generated (e.g., molecular diagrams and animations) and generated by probes connected to student experiments (e.g., tabular data and real time graphs). Students work in a networked environment to comment and build on each other's work.
http://www.chemsense.org/
Contact: Robert Kozma, robert.kozma@sri.com

Integrated Molecular Visualization

As the wealth of molecular information existing in public and private databases or derived from tools based on new technologies continues to grow, the need to see and integrate results is now more important than ever. MSI is developing programs that facilitate understanding through effective visual representation, and provides tools for integrating chemistry on the PC.
http://www.accelrys.com/
Contact: John Wintersteen, johnw@msi.com

Chemical Computing Groups software MOE and Proteins: Structure, Function and Dynamics CD

Two powerful visualization tools designed for scientific research are used by students in upper division chemistry courses.
http://alpha1.chemistry.duq.edu/moe_faq.htm
Contact: Jeffry Madura, madura@duq.edu

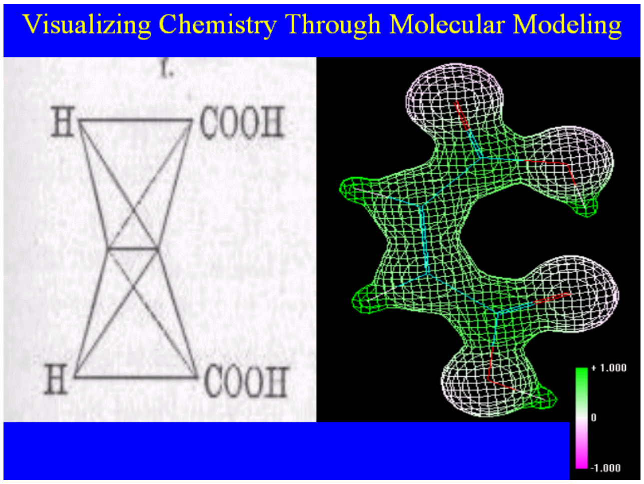
Quantum Explorer

The Quantum Explorer programs are intended to provide students with a first introduction to the way that molecules are built from atoms. The programs are in 2D and 3D and extend from models of atomic structure, to diatomic atoms, and finally to representations of polyatomic molecules.
http://qsad.bu.edu
Contact: Peter Garik, garik@bu.edu

ChemViz -- A free WWW-based resource for high school teachers and students

NCSA ChemViz has been available for over eight years to high school students and teachers, allowing them to explore more sophisticated models for atoms and molecules. The goal has been to provide powerful computational opportunities so that students can use the same type of tools that working scientists use to visualize difficult atomic and molecular models.
http://chemviz.ncsa.uiuc.edu/
Contact: Barry Rowe, roweba@cmi.k12.il.us

Visualizing chemistry for majors and non-majors through molecular modeling



At The King's University College, chemistry students are introduced in their first year to HyperChem 5.1, a comprehensive PC-based molecular modeling software package. Molecular modeling is then used across the chemistry curriculum to visualize three-dimensional structures, understand molecular geometry and properties, visualize molecular orbitals and bonding, carry out thermodynamic calculations and conformational analysis, understand electronic and vibrational spectroscopy, and visualize simple reactions with molecular dynamics. Molecular modeling is used along with experimental findings in investigative projects.
Contact: Peter Mahaffy, pmahaffy@KingsU.ab.ca

Interaction and Assignability

Software has been developed to engage students in their work with animations of molecular reaction mechanisms, moving toward a student-active approach to visualization. Letter-line drawings are used instead of 3D models as tools for following electron flow in organic mechanisms. The UMass OWL system, a web-based homework and tutoring system, is being extended for use with molecular models.
http://soulcatcher.chem.umass.edu/
Contact: Bill Vining, vining@soulcatcher.chem.umass.edu

Oslet

Oslet is a molecular simulation software being developed at the Concord Consortium. Oslet can be used to build arbitrary 2D (for the time being) atomic- scale models ranging from gas, solids, surfaces, molecules to polymers, micelles and bilayers, run them using molecular dynamics engines, and analyze the results. Oslet differs from some existing molecular dynamics software in the fact that it can not only do particle dynamics (typically with the Lennard-Jones potentials), but also build any kind of 2D molecular structure and investigate its dynamical behaviors. Oslet has a powerful modelling environment with which the user can create and edit a structure.
http://www.concord.org/%7Ebarbara/workbenchcc/workbench_index.html
Contact: Bob Tinker and Qian Xie, qxie@notes.concord.org

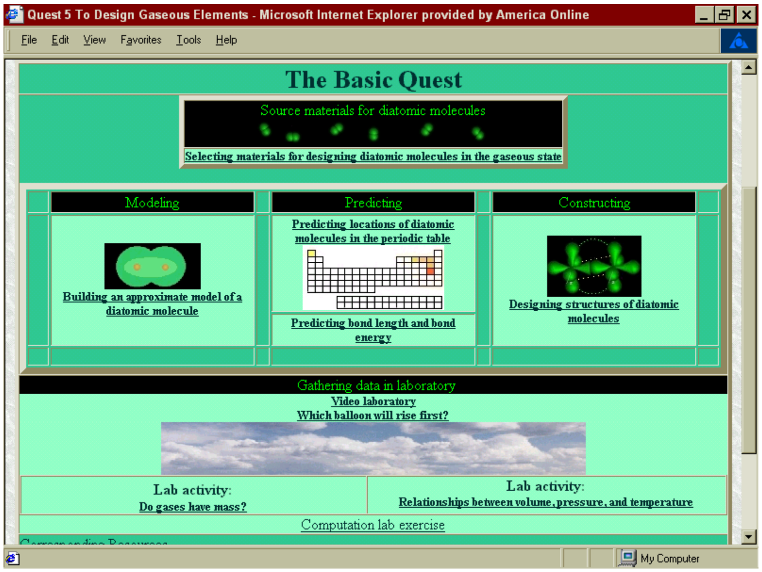
A Web-based Molecular Level Inquiry Laboratory Activity

A new computer-based atomic level simulation of an ideal gas was written in JAVA and is accessed by students through a web browser. This software is used in conjunction with a laboratory experiment report developed within the framework of an inquiry instructional strategy. This molecular level laboratory experiment is used in combination with a parallel macroscopic laboratory experiment. It is hypothesized that students exposed to these kinds of parallel activities will be better able to link their macroscopic, microscopic, and symbolic understanding of chemical concepts.
Contact: John Gelder, jgelder@okstate.edu

The Consortium for Technology in Teaching Chemistry, (CTTC) Program at USC

The CTTC was started last year to establish a consortium for Southern California teachers and institutions who are interested in implementing computer technologies in their high school science classrooms, in order to pool resources, share ideas, develop strategies, and provide continuing education. Atomistic and molecular imaging using STM and AFM are used to visualize chemistry and materials.
http://michele.usc.edu/cttc/index.html
Contact: Bruce Koel, koel@chem1.usc.edu

ChemDiscovery



ChemDiscovery uses a design approach to teach chemistry. It consists of a series of computer-based projects, called quests, that assist students in designing a virtual picture of the world from a chemical perspective. In ChemDiscovery students construct individual learning pathways. As students work through each quest, they choose source material, design nuclei, atoms, ions, molecules, and reactions, predict the properties of the objects they have designed, construct the objects, and check their predictions.

www.unco.edu/chemquest/mission.htm

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Additional Relevant Web Links

Workshop on modeling and visualization in teacher education
http://www.eot.org/edgrid/mvworkshop.html

NCSA virtual reality demos (Note: most require special hardware)
http://www.ncsa.uiuc.edu/VEG/homepages/tcoffin/ACCESS/access_demos.html

Virtual molecular dynamics lab
http://polymer.bu.edu/vmdl/

Protein explorer
http://proteinexplorer.org

List of Molecular Visualization sites
http://molvisindex.org

Leffingwell's list of visualization resources
www.leffingwell.com/links4.htm

Computational Chemistry for Chemistry Educators
http://www.shodor.org/compchem/

Cabrillo College molecular visualization page
http://c4.cabrillo.cc.ca.us/

Okanagan University's collection of viewable molecular models
http://www.sci.ouc.bc.ca/chem/molecule/molecule.html

Indiana University's Molecular Structure Center
http://www.iumsc.indiana.edu/common/common.html

MacMolecule and PCMolecule home page
http://www.molvent.com/

Home page for Chime
http://www.mdli.com/chemscape/chime/

Home page for Rasmol
http://www.umass.edu/microbio/rasmol/

PDB Lite molecule finder
http://pdblite.org

The Role of Representations in Problem Solving in Chemistry, George M. Bodner and Daniel S. Domin
www.inform.umd.edu/EdRes/Topic/Chemistry/ChemConference/ChemConf96/Bodner/Paper2.html

Recent Applications of Hyperactive Chemistry and the World-Wide-Web, Henry Rzepa
http://www.ch.ic.ac.uk/rzepa/cc96/

Are Simulations Just a Subsitute for Reality?, Harry E. Pence
http://snyoneab.oneonta.edu/~pencehe/paper9CC97.html

Using Technology to Solve the Conceptual Riddle: "How can we help them see what we see?" Jimmy Reeves
http://aa.uncwil.edu/reeves/confchem_2000/

Why use animations and simulations? Brian Pankuch
http://www.ched-ccce.org/confchem/2000/b/pankuch/uses.htm

Computer Animations and Simulations in General Chemistry, Chung Chieh and Newman K.S. Sze
http://www.science.uwaterloo.ca/~cchieh/cact/trios/simulation.html

Discovery-based General Chemistry Using Chemland Simulations, Bill Vining
http://www.ched-ccce.org/confchem/2000/b/vining/vining.htm

Using Simulations to Transform the Nature of Chemistry Homework, David Yaron, Rea Freeland, Donovan Lange, and Jeff Milton
http://www.ched-ccce.org/confchem/2000/b/yaron/Default.htm

Assessing modelling capability in chemistry, John Oversby
http://www.ched-ccce.org/confchem/2000/c/oversby/oversby1.html

Quantum Sciences across Disciplines:
http://qsad.bu.edu

An Introduction to Chemistry on the Internet
http://chemlinks.beloit.edu/MolecularModel/internet.html

Chemistry Visualization Resources for Teachers
http://www.canby.com/hemphill/chmvis.htm