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CHAPTER 6

TEACHING AND LEARNING WITH THREE-DIMENSIONAL REPRESENTATIONS

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Abstract. Computer-based visualizations play a profoundly important role in chemistry instruction. In this chapter, we review the role of visualization tools and possible ways in which they may influence thinking about chemistry. There are now several visualization systems available that allow students to manipulate important variables in obtain a solution to a scientific problem. We discuss the fundamental differences between these tools, and we emphasize the use of each within the context of constructivist curricula and pedagogies. We also consider the impact such tools may have on visuo-spatial thinking. We suggest that although visuo-spatial ability may be important in visualization use, its role has at times been overemphasized. We argue for a more nuanced, richer understanding of the many ways in which visuo-spatial reasoning is used in solving chemistry problems. This discussion leads to a set of design principles for the use of visualization tools in teaching chemistry. Finally, we present our work on the Kinemage Authorship Project, a program designed to assist students in understanding spatial structures in complex, biochemical molecules. The Kinemage Authorship Project allows students to construct their own molecular visualizations, and we discuss how this may lead to greater understanding of the spatial properties of molecules. This constructivist program embodies many of the design principles that we present earlier in the chapter.

INTRODUCTION

Visualization tools are among the most important technologies for learning at the high school and undergraduate levels. Educational researchers have devoted considerable effort to the refinement and implementation of visualization tools for science students because of the important role of perceiving, understanding and manipulating three-dimensional spatial relationships for learning and problem solving in many sciences. Although such tools exist for most sciences, chemists and biologists have been among the strongest advocates for visualization tools because their disciplines require the conception of multiple, complex three-dimensional spatial relationships both within and between molecular structures. Repeatedly, instructors find that their students have great difficulty understanding these relationships in these domains, which many novel visualization tools aim to make more comprehensible (Copolo & Hounshell, 1995; Habraken, 1996; Wu, Krajcik, & Soloway, 2001).

In this chapter, we will explore the potential benefits of visualization tools in the teaching and learning of science at the secondary and post-secondary levels. We discuss the advantages of using these tools in conjunction with constructivist

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pedagogies. We also propose new approaches to investigating their effectiveness as learning aids by focusing on cognitive models of visualization. We detail one novel constructivist visualization-based curriculum that uses *Kinemage* to teach undergraduate biochemistry students concepts of enzyme structure and chemical reactivity. We conclude with a discussion of the opportunities and novel research directions that using a cognitive framework to explore visualization tools can engender.

VISUALIZATION IN THE SCIENCE CLASSROOM

Visualization is universal to the science classroom regardless of domain or level; however, the underlying need for visualization varies with the topic of study. In geology, students must comprehend the spatial relationships between different earth structures that are not perceptually accessible due to both their macroscopic size and their location beneath the crust of the Earth. Visualizing geological structures is complicated because these structures seem ostensibly static, but students must perceive that the structures are actually dynamic objects that move on a time-scale many orders of magnitude greater than that of daily human life. In physics, students perform similar mental feats of visualization that have their own special challenges. Physics students must perceive the spatial relationships between the interaction of forces that result from phenomena such as tension, friction, gravity, and electromagnetism. Because these forces have no visual manifestation that students can perceive, visualization is equally critical for understanding in this domain.

Both instructors and practicing scientists are quick to point out that a critical component to problem solving and comprehension in the sciences lies in a student's ability to visualize the spatial relationships, and transformations of those relationships, among various phenomena or structures. Consequently, many believe that it is critical for a student to generate a mental model of the scientific phenomena under study. In geology, a student might need to visualize how two plates in the Earth's crust slide against one another and what effect the movement has on the surrounding landscape. In physics, a student might imagine mental models of force vectors acting on a vehicle and how manipulating the magnitude of any one vector can alter the vehicle's velocity. Because students have no basis for generating mental models of these phenomena from their everyday experience, instructors provide their students with a plethora of diagrams, models and pictures to assist the visualization process. Unfortunately, the two-dimensional representations commonly used in the science classroom can only approximate the three-dimensional events they represent. This limitation can distort the mental images that students attempt to visualize and hinder learning.

To say that visualization is important for learning in the chemical sciences glosses over the fundamental role that these cognitive processes play at all levels of study in these domains. For example, understanding the nature and importance of spatial relationships is only the most basic component of spatial cognition in the chemical sciences. As students' studies advance, comprehending the particular details of spatial relationships in relevant diagrams, models, and images becomes increasingly important. Not only must students be aware that such relationships exist, but they must also apprehend the particular constraints that molecular structure can have on the macroscopic shape of a substance and the role that these constraints play on molecular interactions and chemical reactivity. While the task may be simpler for small molecules composed of five or fewer atoms, it becomes considerably more difficult when students must deal with biological molecules that can contain thousands of atoms, each of which possesses a unique relationship with the others. For example, when considering a large enzymatic molecule, a student might be required to understand how the position of one particular oxygen atom affects the relationship between thousands of other atoms in the enzyme and how that shape controls the enzyme's chemical activity. To understand this, the student must consider—often simultaneously—properties such as bond angle, bond length, orbital shape, connectivity and chirality, to name a few characteristics.

Particularly in the chemistry classroom, traditional instruction may inhibit or complicate the necessary understanding because it relies on two-dimensional diagrams to represent three-dimensional molecular structures. Although instructors and practitioners are adept at the selection and use of different two-dimensional representations to describe three-dimensional molecular structures, students are rarely successful at interpreting or manipulating the wide variety of representations available (Keig & Rubba, 1993; Kozma, Chin, Russell, & Marx, 2000). For instance, students often report great difficulty understanding that the Fischer projection in Figure 1 represents the same molecule that the ball-and-stick model represents. Although the ball-and-stick model emphasizes the three-dimensional relationships between atoms in the molecule, the Fischer Projection emphasizes the connectivity between the atoms; one must understand the formalisms of the representation to perceive the three-dimensional relationships that are embedded in the two-dimensional diagram. Although the representations in Figure 1 are often restricted to organic chemistry classrooms, the difficulty in perceiving and understanding three-dimensional relationships is ubiquitous among both advanced undergraduate students and novice high school students (Johnstone, 1993).

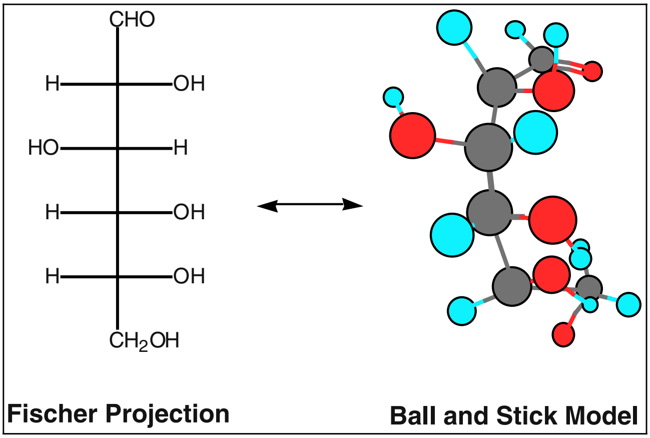

Figure 1. *Unlike ball-and-stick models, Fischer projections obscure three-dimensional spatial relationships and instead highlight atom connectivity, which students find difficult to perceive.*

SUPPORTING VISUALIZATION WITH VISUALIZATION TOOLS

Educational researchers have recently begun to concentrate on the development of a wide variety of visualization tools and novel pedagogies to aid students in science learning at all levels. These tools describe a spectrum of learning environments that support many different types of visualization from concretizing abstract concepts to understanding spatial relationships. Tools are now available that allow students to visualize experimental data sets, simulate experiments, or construct models of imperceptible entities. At their core, each of these tools presents students and instructors with several unique opportunities for teaching and learning science that allow students to visualize complex relationships directly from computer-generated visualizations. Advocates for the use of visualization tools can be found among science teachers at all levels. High-school teachers report that students gain a more robust conceptual understanding of classroom content when their lessons are supported by the use of visualization tools (Copolo & Hounshell, 1995; Wu et al., 2001). Likewise, college teachers have reported similar benefits and support incorporating these visualization tools to enrich traditional pedagogies (Crouch, Holden, & Samet, 1996). In fact, CD-ROMS with visualization tools are packaged with many science textbooks, particular for undergraduate chemistry. Given the compatibility and small disk space required by these programs, a single CD-ROM can support instruction with tools that animate textbook diagrams, model virtual laboratories, and supplement classroom lectures with interactive tutorials.

Visualization tools to enhance teaching and learning in the sciences fall roughly into two groups. The first, which we label *content-specific tools*, accounts for the majority of visualization tools currently in use. Content-specific tools are stand-alone programs that teach specific concepts in a particular science. The other group, which we label *general learning environments,* are general-purpose programs that can be used across a variety of scientific domains. Both categories of visualization tools present unique opportunities to students and instructors in the science classroom. These opportunities are as varied as the tools that have been developed: instructors can use them as simple visual aids to support a lecture or they may fundamentally alter the nature of their teaching by allowing students to explore the tools with little guidance. In essence, each of these tools, regardless of form, attempts to improve learning by visually representing scientific phenomena in conjunction with or in place of text-based descriptions or symbolic notations.

There are, however, fundamental differences between the goals that motivate the two types of visualization tools. Those who favor general learning environments advocate the development of open-ended tools, which instructors can modify easily to tailor the learning experience for many different science classrooms as well as for individual students. These modeling environments emphasize multiple representations of concepts, flexible interfaces, broad functionality, and a strong interactive component (Wilensky, 2001). General learning environments present an alternative to direct instruction by giving students opportunities to explore fully developed models to discover scientific principles. Most general learning environments also allow students to alter given models, or to develop their own, with or without instructor support.

One such environment, *NetLogo,* is based on the assumption that students learn better by connecting the visual representations of microscopic phenomena with macroscopic domain concepts that can often be represented graphically (Wilensky & Resnick, 1999). Educational researchers, in conjunction with instructors and students, have used the NetLogo modeling environment to model and teach phenomena in biology (Centola, Wilensky, & McKenzie, 2000), physics (Wilensky, 1999), and chemistry (Stieff & Wilensky, 2003). Students have used the visual representation of microscopic phenomena, be they molecules, mammalian cells, or gas particles, to deduce fundamental concepts, such as chemical equilibrium, asexual reproduction, or Brownian motion. The NetLogo environment attempts to simulate physical reality with a high degree of fidelity and provides students with direct access to the programming code that controls each model so that they can understand the relationship between the virtual world and the world it represents.

A unique implementation of NetLogo, entitled GasLab, illustrates the goal of this class of visualization tools. GasLab allows students to explore a virtual environment of gas particles in a box to discover the relationship between a visual representation of gas particles in motion, a speed histogram, and a kinetic energy histogram to learn about the cause and effect of the Maxwell-Boltzmann distribution (Wilensky & Resnick, 1999). As the dynamic simulation runs, students are able to observe the visual representation, in which particles constantly collide and transfer energy. Histograms of speed and energy are reported simultaneously, and the student can discern that the total energy of the system maintains an equilibrated distribution. Together, the three representations (illustrated in Figure 2) allow students to develop a richer understanding of the connection between the physical phenomena of particle motion and collisions, the concepts of energy and temperature, and graphical representations of non-normal distributions.

In the geosciences, the development of visualization tools has also focused on providing students with detailed visual representations of domain concepts in the same spirit of tools like NetLogo. Unlike general-purpose modeling environments these tools, such as WorldWatcher (Edelson, Gordin, & Pea, 1999) and Geo3D (Kali & Orion, 1997), have been designed specifically for the purpose of providing students with visual representations of phenomena and concepts in climatology and geology, respectively. Instructors and researchers alike have praised the tools because they show students complex geological structures that are not observable directly due to their macroscopic structure. These tools also allow students to perceive the relationship between different spatial transformations of geological structures as they occur over time. This feature is particular important because study in these domains often require students to comprehend the transformation of the phenomena under study on multiple time scales. For instances, students might need to reason how local albedo or plate tectonics as they transform over a few seconds and over hundreds of years. Reportedly, the dimension of time adds considerable difficulty to students' ability to visualize such phenomena (Kali, 2003). Moreover, verbal descriptions or static diagrams of dynamic relationships can result in significant misconceptions among students, which makes these tools particularly valuable (Kozma & Russell, 1997; Stieff & Wilensky, 2003).

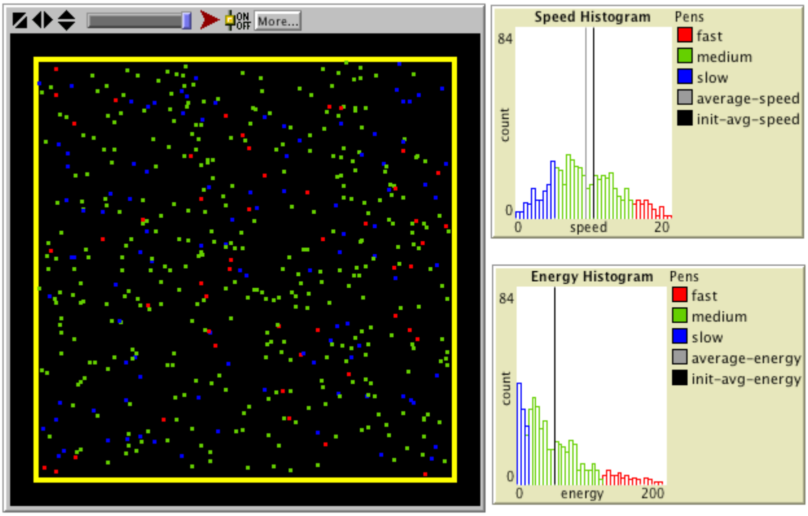

Figure 2. *The NetLogo modeling environment supports the GasLab curriculum that teaches students the relationship between particle motion and the distribution of kinetic energy. A color version of Fig. 2 is given in the Colour Section.*

Many of visualization tools allow students to compare concept maps with visualizations of actual geological data to enrich the learning experience. Figure 3 illustrates how the WorldWatcher interface accomplishes this goal by focusing on the relationship between surface temperature and location on the Earth. With the aid of a visualization of average surface temperatures across the planet, students engage in an investigation to discover how the nature of incoming solar radiation results in different climates. WorldWatcher is equipped with an extensive dataset that allows students to compare temperature data from many different years that climatologists have collected in the field. Using this data, students are able to construct explanations of climate and geography from their own investigations instead of learning them from direct instruction.

In the chemical sciences, educational researchers have focused much of their efforts on the development of visualization tools that allow students to visualize the three-dimensional spatial relationships that are embedded in traditional two-dimensional molecular representations. The tools emphasize how students can learn fundamental domain concepts by understanding the three-dimensional shape and structure of molecules. For example, these tools can help students in molecular biology courses visualize the shape of proteins on the surface of a white blood cell that give the cell the ability to detect and destroy bacteria and viruses. Visualization tools for the chemical sciences often aim at the secondary goal of teaching students the relationships between the different two-dimensional diagrams that domain practitioners most commonly employ. The tools are designed to help students see the relationships among the various two-dimensional diagrams. Students use them to underscore that even though different two-dimensional representations of the same molecule may appear disparate, each represents the same three-dimensional structure.

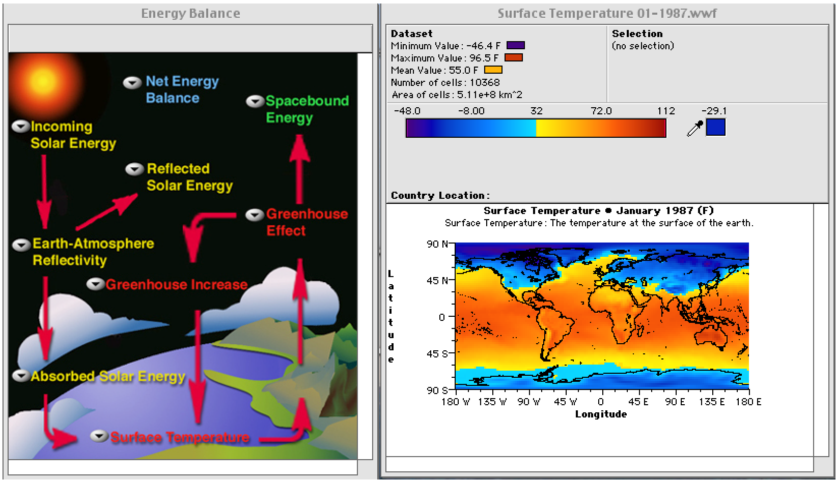

Figure 3. *The WorldWatcher visualization tool allows students to compare concept maps with visualizations of real scientific data in a guided inquiry environment. A color version of Fig. 3 is given in the Colour Section.*

One such visualization tool, eChem (Wu et al., 2001), is designed to allow students to compare two-dimensional diagrams with three-dimensional visualizations to learn organic chemistry. Students can use the tool to construct virtual models of small organic molecules using several common molecular representations (see Figure 4). The tool allows students to compare space-filling models, ball-and-stick models, and wire-frame models vis-à-vis to learn how atomic constituency and connectivity relate to the overall size, shape, and structure of a molecule. The tool also provides students with a database of physical properties for several common molecules. With this information, students can deduce how the size and shape of molecules affect properties such as boiling point, density, hardness, and solubility.

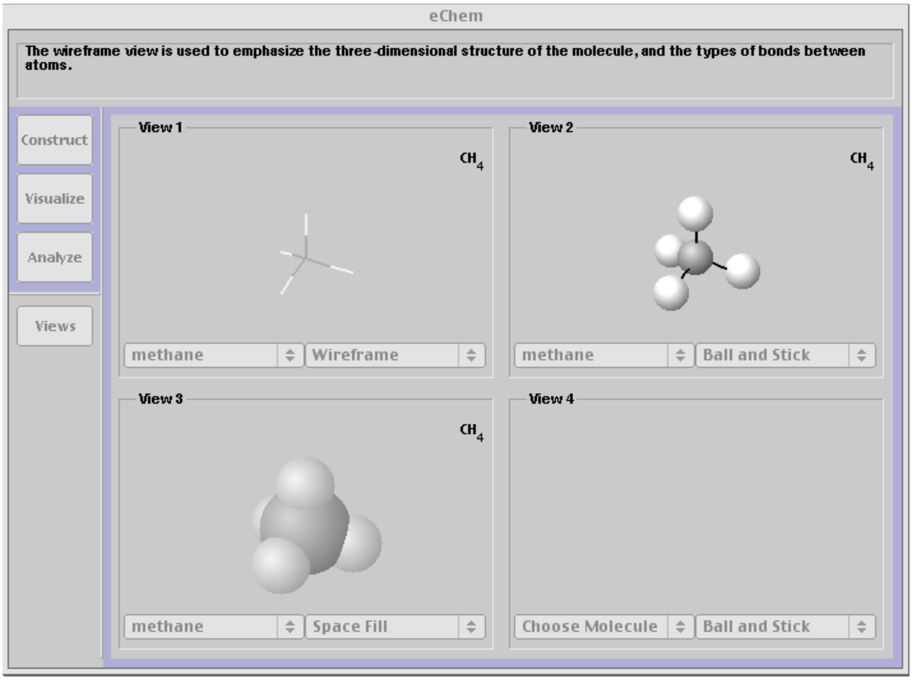

Figure 4. *The eChem visualization tool allows students to compare three-dimensional and two-dimensional representations to better comprehend structure and reactivity.*

TOWARDS A THEORY OF EFFECTIVE VISUALIZATION USE

Although the research community generally agrees that visualization tools are a boon to science education, most of the enthusiasm is based more on anecdotes than on evidence (Horowitz, 2002). In part, the scarcity of data supporting the use of visualization tools is due to the rapid growth in the number and diversity of tools. Many educational researchers and software designers continue to focus their efforts on honing interfaces and constructing curricula that take advantage of visualization tools before turning their attention to gather data on the impact of the tools. In addition, the wide variety of tools available presents a daunting analysis task for the few researchers currently investigating their efficacy. Consequently, relatively little work exists that assess the impact of such tools on both learning outcomes and pedagogy. Despite the paucity of evidence, however, a few studies have aimed to measure the learning outcomes from their use.

The developers of visualization tools have, themselves, conducted the majority of the research on the effectiveness of their tools, and they have reported a wide range of findings on the efficacy of specific pieces of software. Unavoidably, the designers have conducted their studies in conjunction with the ongoing development of a particular tool. Because of this, their research methods have often been hindered by the lack of a fully functional tool. Although many of these studies have been limited to anecdotal reports about student attitudes and understanding, the findings have begun to indicate positive outcomes from each implementation (Crouch et al., 1996; Wu et al., 2001). Very few studies have attempted to document the impact of their curricula on larger groups of students with more rigorous methods. While these few studies produced some supporting evidence for the anecdotal reports, they have mostly relied on pre- and post-test measures from traditional curricula (e.g., Ealy, 1999; Noh & Scharmann, 1997). In general the limited amount of evidence has been favorable, although some designers have observed declines in problem-solving ability among students who have learned using visualization software (Copolo & Hounshell, 1995). Clearly there is a strong need for research to overcome the empirical limitations regarding the use and effectiveness of visualization tools in science education.

Perhaps more importantly, we lack clear theoretical perspectives to motivate the role of visualization strategies and the effectiveness of visualization tools. There are, of course, suggestions as to why visualization tools do or do not work, but these have not been integrated into a coherent theoretical account of why visualization tools are likely (or unlikely) to help students learn in a given science domain. We need now to integrate these various suggestions into a coherent theoretical account of visualization use and comprehension. New theoretical models of visualization as a cognitive skill for learning and problem solving must replace general assumptions about the critical role of visualization in the sciences. In parallel, new research methods that both determine empirically the role of visualization in learning science and provide detailed descriptions of the quality of learning with novel visualization tools must replace marginal pre- and post-test measures and imprecise anecdotal self-reports. Collaborations between educational researchers, designers, cognitive science, and science practitioners are critical to the development and success of these new theories and methodologies. Members from each of these groups provide valuable input on the role, implementation and value of visualization tools as joint members of the science education community.

Our work ultimately is aimed at these general goals, particularly for visualization tools that teach using three-dimensional representations in the chemical sciences. Perhaps more than any other science domain, the chemical sciences have garnered strong advocates for the use of visualization strategies and visualization tools based on the simple assumption that visualization is critical because the molecular world is three-dimensional (Habraken, 1996). We seek to develop a theoretical framework to replace this assumption regarding the use of visualization tools for the chemical sciences that is motivated by principles and research from cognitive science and the larger science education community. Joint efforts to develop new visualization tools, theoretical models, and research methods have been effectively established to study learning in physics (Sherin, diSessa, & Hammer, 1993) and geology (Keating, Barnett, Barab, & Hay, 2002), but are lacking in the chemical sciences. In the following sections, we present three principles of a theoretical framework that aims to motivate the use of visualization tools and specify the role of visualization as a cognitive strategy in the chemical sciences. Although these principles are not exhaustive, we offer them as a starting point for further research on visualization by the science education community.

Principle 1: Design Visualization Tools for Chemistry to Support Spatial Cognition

Chemistry has always been a very visually oriented science, and novel visualization tools should support students' understanding of the variety of visual representations of chemical compounds and reactions. As mentioned above, the representation of chemical structures at the molecular level is particularly important because of the direct relationship between the structure, the chemical reactivity, and the physical properties of a compound. There are limitless examples of this: the arrangement of individual atoms in a semiconductor is directly related to the semiconductor's ability to conduct electricity, the bonding pattern of carbon atoms in a diamond is responsible for the gem's extreme hardness, the interactions between water molecules in ice results in the shape of snowflakes. All chemists are familiar with these relationships and consider them of primary importance in most courses related to the chemical sciences.

In particular, study in this domain requires that students gain a strong understanding of the concept of stereochemistry. This concept concerns the connectivity and three-dimensional spatial arrangement of atoms within an individual molecule. Even relatively small molecules, such as amino acids, have multiple spatial arrangements that can result in different *stereoisomers*, which are unique molecules that are composed of the same atoms. Understanding the structure and relationship between stereoisomers is crucial to the basic and advanced study of chemistry. In introductory courses, students must know how to name and build each isomer. In advanced biochemistry courses, students must understand how different stereoisomers create different proteins with different functions. For example, only one stereoisomer of amino acids, known as the L isomer, is found in proteins in living systems; incorporation of the R isomer into a protein can a have disastrous impact on biological function. A protein containing a single amino acid of the alternate arrangement could well be dysfunctional and result in systemic disease at the organism-level. Figure 5 illustrates the minor difference in spatial arrangement between the stereoisomers for the amino acid, alanine. Note that although both molecules in the figure contain the same number and type of atoms, they are mirror reflections of one another that cannot be superimposed; consequently, they are unique stereoisomers.

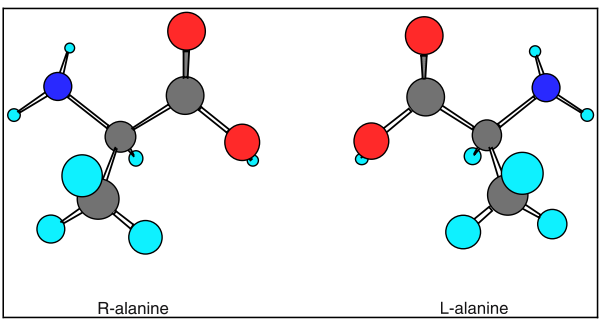

Figure 5. *The two stereoisomers of alanine are composed of the same atoms, but each has a unique spatial arrangements.*

Students must become adept at not only perceiving the spatial relationships between stereoisomers but also at manipulating them as needed to solve problems in the classroom and the laboratory. Two well-known medical examples serve as reminders of the importance of stereochemistry. One unfortunate example concerns a drug, thalidomide, that was given to numerous women in Europe as a treatment for nausea during pregnancy. Although effective, the drug caused severe birth defects. Investigation showed that thalidomide had been synthesized and distributed as a pair of stereoisomers. Only one stereoisomer was responsible for the therapeutic effects of the drug; the other stereoisomer caused the serious side effects. Thalidomide was quickly banned as an antinauseant banned because of its side effects, but today medicinal chemists are now testing the therapeutic stereoisomer as an anticancer agent. The second example reveals the importance of understanding stereochemistry for diagnosing disease. Sickle cell anemia is caused by single amino acid replacement mutation in the protein hemoglobin. This mutation places an incorrect amino acid in a critical position on the surface of hemoglobin that causes the protein molecules to stick together and form long, insoluble fibers. These insoluble fibers distort the red blood cells and give them the characteristic “sickle” shape after which the disease is named. Understanding the relationship between the structure of the mutated protein and the depleted function of the diseased red blood cells has provided new avenues of research toward treatments for the disease.

It is important, then, for chemists and biochemists to be able to visualize the spatial arrangement and connectivity between atoms in molecules both small and large. Chemists have traditionally used molecular models to help students visualize the proper mental image of molecules and their interactions. Typically, these models are the plastic ball-and-stick modeling kits that are familiar to anyone who has taken a chemistry course. Other chemists have used balloons to illustrate atomic orbitals or inverted music stands to show displacement reactions. Unfortunately, these models are static in nature and do not allow students to see dynamic interactions between molecular structures. Indeed, some students can come to believe that molecular bonds exist as rods that hold nuclei together in the same way that the plastic pieces connect the pieces of the modeling kit. These types of models work well for small molecules and give the student a tactile way to approach their formulation of a mental model, but many students often fail to understand the relationship between the models, diagrams, and real molecules (Keig & Rubba, 1993; Wu et al., 2001).

Visualization tools stand to aid students’ perception and mental manipulation of three-dimensional relationships by providing virtual models of actual molecular structures that maintain a high degree of fidelity with real molecules. Such tools give students direct access to authentic representations of the phenomena under study in the chemical sciences. Designers of educational software for chemistry have already realized the potential of visualization software to provide rich details about shape and structure of the molecules for advanced research, and we believe this same potential applies to the chemistry classroom. These tools provide students with the ability to compare different stereoisomers, to learn techniques for translating one molecular representation into another, and to construct models of molecule interactions and subsequent chemical reactions. Moreover, we suggest that there the use of visualizations may benefit students in ways that extend beyond the benefits that have been assumed.

As we continue to develop visualization tools, the generic goal of using them to help students appreciate the overall size, shape and structure of particular molecules is insufficient. Instead, we must focus our designs in such away that students learn to use such tools to directly support visualization strategies on appropriate tasks. That is to say, dynamic visualization tools allow students to manipulate virtual molecules in much the same way they might manipulate a mental model of a chemical reaction. Therefore, productive tools should offer users the capability to rotate molecules to gain new perspectives or viewing angles of molecular structures in isolation or interaction. Additional features that allow students to rotate individual bonds within a molecule to see how the overall shape of a structure changes as a consequence provide even more versatility and authenticity. For example, students might use them as researchers do to learn about DNA structure by constructing a visualization to illustrate how replacing one DNA base-pair with another can distort the double helix. Each of these capabilities of visualization tools provides an advanced external representation with which students can perceive and manipulate spatial transformations during problem solving. These transformations are nontrivial and even the most adept students stand to benefit from the use of a tool to assist in visualizing them.

Principle 2: Investigate the Role and Efficacy of Visualization Tools with Cognitive Models

The prior section suggested that a mental visualization is perhaps the key to success in chemistry and hence should be the cornerstone for the development of visualization tools. Many authors have taken this approach, suggesting that visualization alone is the most important predictor of success in chemistry. Traditionally, many researchers have cited a student's inability to visualize the three-dimensional structure embedded in two-dimensional representations as the primary barrier to learning. Although some have suggested that the barrier results from the total amount of information that each particular representation contains (Keig & Rubba, 1993; Kozma et al., 2000; Stieff & Wilensky, 2003), most researchers have repeatedly emphasized that it is the spatial information, in particular, embedded within each representation that confuses students (Bodner & Guay, 1997; Brownlow & Miderski, 2001; Carter, LaRussa, & Bodner, 1987; Coleman & Gotch, 1998). The latter group of researchers emphasizes that the three-dimensional structure of a molecule plays a large role in the molecule's properties and reactivity, and they suggest that students must stay mindful of these features in order to understand and complete most chemistry tasks. These claims have been made largely independent of the level of instruction or the topic of discussion: chemistry education researchers have made the case for the role of visualization in learning chemistry equally for both secondary students of general chemistry and for undergraduate students of organic chemistry.

We agree that the abilities to perceive and understand three-dimensional spatial relationships are important for many science domains, particularly chemistry, but the precise role of such abilities in these domains is relatively unclear. Assumptions that postulate a central role of visualization in the sciences on the simple observation that these domains concern imperceptible three-dimensional objects fail to consider the complex interaction between visualization, spatial reasoning, and external representations of spatial information. Perhaps more problematic is that such assumptions disregard the unique details of individual tasks, which may be essentially unrelated to the representations or the spatial information present in the task. For example, consider a task from an organic chemistry classroom that concerns the reaction between two large, spatially-complex molecules that produces two new molecules. At first, it may appear that students with well-honed visuo-spatial abilities would be predisposed to excel on this task. However, further inspection of the task reveals that it simply requires the student to determine the relative ratio of each molecule in solution after the reaction concludes. Therefore, despite the presence of molecules with complex and detailed spatial information, the task is fundamentally a math problem contextualized in the chemistry classroom.

As we develop novel visualization tools and curricula for the science classroom, we must develop stronger cognitive models regarding the role of visualization as an aspect of spatial cognition that includes a principled foundation for the use of visualization tools. Instead of simple assumptions, we must base these models and frameworks on research and theoretical principles from cognitive science regarding spatial cognition as a fundamental cognitive strategy. Some earlier research programs attempted to characterize visualization as a form spatial cognition in the chemical sciences by basing their work on the assumption that individual differences in visuo-spatial abilities were an underlying cause of variations in performance. Indeed, those studies found several moderate correlations between measures of visuo-spatial ability and performance; however, the results of such studies were not definitive, and several are quite contradictory (Carter et al., 1987; Ealy, 1999; Keig & Rubba, 1993). Paradoxically, findings from that line of research have revealed that the strongest correlations exist between standardized measures of visuo-spatial ability and performance for chemistry tasks that do not include any spatial information. Although well established, the focus on individual differences has led to the basic claim that students who perform well on standardized measures of visuo-spatial ability also perform well in chemistry and other sciences. This line of research has generated little information regarding the type of cognition underlying learning and problem solving in the chemical sciences.

A more rigorous cognitive model that explicates the form and function of spatial cognition for scientific problem solving can provide a productive theoretical framework for both the design, implementation, and assessment of visualization tools. We advocate a theoretical framework that acknowledges that spatial cognition is neither simple nor uniform. We posit that the role of spatial cognition in problem solving can vary as a function of the demands of a task and the features of the external representations present in the task. At the least, a cognitive model of the role of visualization tools for learning must address two particular features of spatial cognition: the manner in which students encode spatial information and the cognitive strategies with which students manipulate that information.

How Do Students Perceive Spatial Information?

New cognitive models of spatial cognition and visualization tools must first account for research from cognitive science regarding information processing and memory modality. Such work has established that individuals can encode information independent of its modality; that is, individuals do not always visualize mental images of physical objects simply because they are three-dimensional. Instead, individuals can encode information that is superficially spatial in nature (e.g. the shape of an object or the distance between two objects) with both analog and propositional mental representations selectively during problem solving based on problem context (Kosslyn, 1994; Markman, 1999; Pylyshyn, 1981). Information that is encoded analogically, as a mental image, is manipulated and stored in a memory system devoted to the processing of spatial information. This system is distinct from a verbal memory system, which stores information encoded as propositional statements (den Heyer & Barrett, 1971; Finke & Pinker, 1982; Pickering, 2001). To further complicate the issue, a reciprocal relation exists between the two systems. For instance, non-spatial information in the form of words or numbers, can cue the visualization of mental images, such as when individuals compare size and shape given only object names (Shepard & Chipman, 1970). Because of these issues, experiments in spatial cognition are careful to limit the amount of non-spatial information that may facilitate cognitive processes other than spatial cognition (Just & Carpenter, 1987; Shepard & Metzler, 1971). Although many representations contain both spatial and non-spatial features that likely involve both spatial and verbal cognition, chemistry educators have yet to consider the role that each system plays.

This latter finding is particularly relevant to investigations concerning the impact of visualization tools in science learning. Although some chemistry education researchers have suggested the spatial memory system described by psychologists is quite obviously the primary cognitive system required for chemistry thinking (Bodner & McMillen, 1987; Coleman & Gotch, 1998; Habraken, 1996), there are two reasons to suspect that visualization plays a more complex role in the cognition underlying scientific problem solving. First, the use of visualization strategies to encode information and to solve problems decreases with development. By the age of eight, most individuals begin to rely less on the perceptual features of objects and more on the verbal labels that they have given objects (Pickering, 2001). For example, when one considers what groceries one must purchase on a shopping trip, they are more likely to think of the necessary items as a list of food names, than as a list of mental images of each item. Despite their predisposition to encode information verbally, adults are better able to recall items encoded as visual images than as verbal labels, which has been coined the *picture-superiorty effect* (Madigan, 1983; Paivio, 1986). Because of the increased dependence on verbal labels for problem solving among adults, the extent to which visualization plays a role in problem solving in chemistry, or any other discipline, becomes an empirical question.

The fact that many molecular representations contain both spatial and verbal information suggests that they require a cooperative effort between both verbal and visual memory. Adolescents' and adults' preference for verbal encoding may increase the difficulty of problem solving in a science domain that requires the student to visualize to effectively problem solve. If this is the case, then the use of visualization tools to reinforce the encoding and manipulation of a mental image of molecular representations could provide substantial support to the science student.

The precise role of the tool to support visualization in this way requires further investigation.

How Do Students Manipulate Spatial Information?

A novel cognitive model must not only determine how visualization tools help students encode visually represented information, they must also determine how the tool affects the cognitive strategies that students use to manipulate that information. Research in cognitive science has shown that alternative strategies are available based on the nature of visually represented information, but the impact of these strategies for problem solving in science remains unknown. Early work in this area established that the visualization of mental images was a crucial strategy for encoding and comparing different representations of three-dimensional objects (Shepard & Metzler, 1971). In those early studies, participants were required to view pairs of three-dimensional shapes (see Figure 6) and asked to determine if the shapes were identical to one another or mirror images. The results of the study revealed that participants required more time to compare the shapes, on average, as the angular disparity between the shapes increased. The linear relationship has repeatedly been interpreted as evidence that individuals visualize and manipulate mental images to solve most tasks that involve three-dimensional spatial information. The nature of the task in Shepard and Metzler's classical experiment is nearly identical to the stereochemistry tasks required in advanced chemistry studies. Indeed, a replication of Shepard and Metzler's original experimental design using molecular representations revealed the same linear relationship between response time and angular disparity (Stieff, 2004). The finding strongly suggests that students routinely attempt to visualize molecular structures for mental rotation when completing tasks regarding stereochemistry.

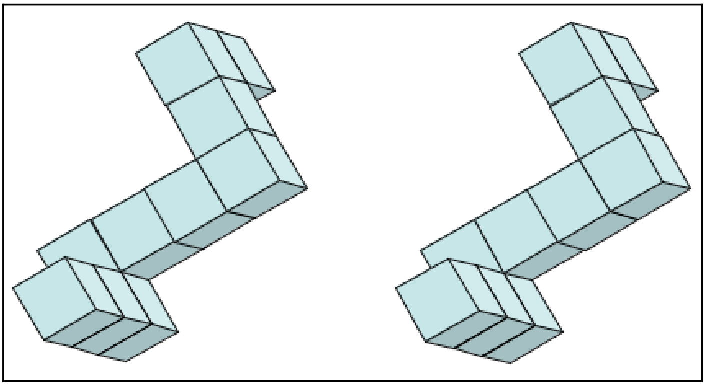

Figure 6. *Individuals are quick to invoke mental imagery strategies to visualize representations of three-dimensional objects*

Although some have suggested the similarity between the laboratory task and stereochemistry problems establishes the primacy of visualization strategies for problem solving in chemistry (Habraken, 1996), additional findings suggest a more nuanced role of visualization strategies in solving stereochemistry problems. Experiments conducted after Shepard and Metzler's original work revealed that mental rotation is a more complicated process than previously assumed. For example, people do not use mental rotation to solve all problems that involve mental comparison of spatial figures. In fact, they seem to rely on mental rotation only for objects that are not rich in information. That is, when comparing generic three-dimensional objects, individuals are quick to use mental imagery and mental rotation to compare objects such as those in Figure 6. However, Just and Carpenter (1987) showed that a very different process is used for the same objects investigated by Shepard and Metzler, if those objects contain additional information, as simple as alphanumeric characters as shown in Figure 7. When presented with these stimuli, participants in the laboratory experiment abandoned a mental rotation strategy and instead made direct comparisons of the stimuli to problem solve. For example, when comparing the two objects in Figure 7, participants did not attempt to visualize and each shape and perform a Gestalt mental rotation; instead they simply noted if the letter 'F' on each object was identical.

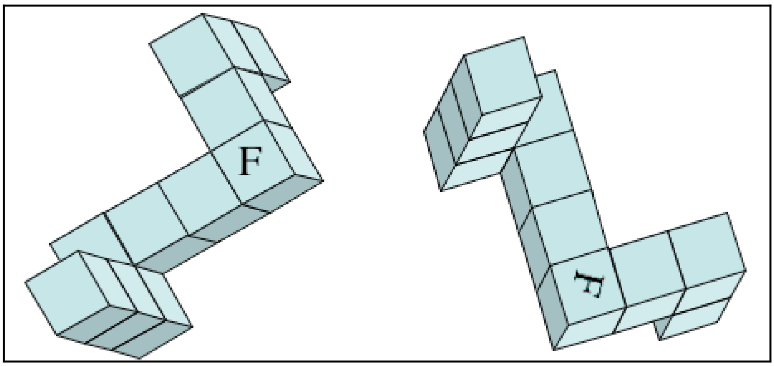

Figure 7. *When comparing "information rich" three-dimensional shapes individuals can avoid visualization and mental rotation.*

Similarly, educational researchers and cognitive scientists have begun to document the use of cognitive strategies alternative to the visualization of mental imagery in science domains even when it is ostensibly required. In mechanical engineering, students have revealed that they can use either mental imagery or invoke abstract rules that obviate visualization to solve tasks regarding gear trains (Hegarty, 1992; Schwartz & Black, 1996). Instead of visualizing a mental animation of a gear train to determine the direction each gear rotates, experienced students can instead invoke a parity rule that states every other gear turns in the same direction. Similarly, science educators have revealed that students use similar abstract rules for solving problems in chemistry. This work has established that students are able to make decisions about stereochemistry by directly inspecting molecular representations without generating a mental image (Stieff, 2004). Instead, the students simply look for planes of symmetry within a molecule to make their decisions. Interestingly, students only apply the rule in limited cases and often resort to visualization when the rule fails to provide an immediate solution. Thus, only when they must treat the molecules as generic objects do students resort to the visualization and mental rotation strategies that Shepard and Metzler described originally.

These findings suggest that more detailed investigations of the use of visualization in the chemical sciences is needed, especially when visualization tools are employed. In particular, the interaction between the use of a visualization strategy and the form of an external representation suggests a nuanced role for visualization tools in the chemistry classroom. We suggest that novel research programs involving the use of visualization tools investigate the varied use of visualization strategies among students without assuming that it is the central cognitive strategy. It must also be made clear how visualization tools alter the form and function of visualization and mental rotation strategies for problem solving in the sciences. The theoretical frameworks and empirical findings from cognitive science suggest that visualization tools have the capability to both enhance and inhibit several aspects of spatial cognition. The extent to which this affects learning and problem solving ability must remain a central feature of novel research programs that hope to use visualization tools more extensively than visual aids.

Principle 3: Implement Tools with Constructivist and Constructionist Pedagogies

Although a variety of novel visualization has developed rapidly in the past decade, concomitant curricula and pedagogies that take advantage of these tools have evolved at a much slower pace. Much to the dismay of the software designers, instructors often fail to incorporate the tools successfully into their classrooms even though many of the tools are available at no cost. In many cases, visualization tools packaged on CD-ROMs and bundled with standard textbooks quickly find their way into the wastebasket instead of the curriculum (Butler & Sellbom, 2002). Educational researchers have cited many reasons for this including a lack of sufficient instructional support, the absence of detailed operating instructions, and a general reluctance of instructors to adopt new tools (Butler & Sellbom, 2002; Duhaney, 2001; Krueger, Hansen, & Smaldino, 2000). Despite the barriers that these factors present to the successful implementation of new visualization tools, both instructors and designer remain committed to overcoming them and to seeking new avenues for successful adoptions.

The design community has advocated that novel science curricula can take full advantage of each of the opportunities that a visualization tool affords by adopting a constructivist approach to teaching and learning (Edelson et al., 1999; Wilensky & Resnick, 1999). Constructivist theories of learning advocate that each student comes to understand scientific concepts based on their individual experiences and their own interpretation of information (Collins, 1996; Papert, 1991; Piaget & Inhelder, 1967). This position stands opposed to the information transmission theories of old that postulate learning takes place when information possessed by the expert instructor is successfully transferred in its entirety to the attentive student. Constructivism acknowledges that individual students can possess different understandings of the same principle that are unique. Although students' individual understandings may differ from the understanding of their instructors, the theory posits that each student can still problem solve and communicate with equal ease. It is important to note that acknowledging alternative understandings does not suggest that all understandings are correct understandings, just that individuals vary in how they apprehend particular concepts.

With regard to visualization tools, a constructivist theory of learning advocates that students learn best when given opportunities to tie together their own knowledge with classroom material to discover or deduce desired principles for themselves (Perkins, 1991). The pedagogy suggested by this tenet of constructivism sharply diverges from didactic or Socratic methods in which instructors lecture to large groups of students about what relevant information must be noted and remembered. In contrast, constructivism takes the position that the latter pedagogies result in poor engagement, low retention, and “inert knowledge” (Brown, Collins, & Duguid, 1989). That is, under traditional instruction students remain passive participants with a tendency to memorize information that they can apply to only the most routine tasks. As such, pedagogical approaches that define the use of visualization tools as simple visual aids to support traditional lectures have little efficacy from the perspective of a constructivist.

Instead, constructivists advocate that students learn through active and varied engagement with visualization tools to maximize their learning benefits. This position takes several different forms, the most popular of which is that of *guided inquiry*. As a pedagogical approach in the science classroom, guided inquiry environments are based on a curriculum in which the student places the role of a research scientist (Edelson, 2001). In the role of a team of scientists, the students receive an authentic scientific problem, which they must solve by designing a research study, collecting and analyzing data with a visualization tool, and presenting their findings to other students. The entire activity is performed under the guidance of the classroom instructor, who helps students make decisions about their study and models the practices of professional scientists. The BGuILE curriculum provides one example of such a guided inquiry environment with the use of data visualization tools, such as *Animal Landlord* and *The Galapagos Finches* (Reiser et al., 2001). BGuILE casts students in the role of field biologists who are attempting to explain such phenomena as food webs and extinction by collecting and analyzing data on climate, animal behavior, and reproduction.

A second pedagogical approach to the use of new visualization tools, which is gaining some precedence in the science education community, is that of *constructionism*. This approach posits that students are better able to apprehend complicated concepts through the act of building their own models of the concepts with the aid of computer-based technologies (Papert, 1991). The constructionist approach specifically supports the use of visualization tools to provide students with opportunities to build models of scientific phenomena in order to increase or improve both learning and problem solving. It is clear that the constructionist approach has particular benefits for courses in the chemistry sciences. In accordance with the tenets of constructionism, students stand best to learn from activities in which they use visualization tools to build models of molecular-level objects and explore their interactions and properties. We suggest that new pedagogical approaches adopt such a pedagogy to provide students with more interactive experiences instead of using visualization tools as a supplemental example of representing the molecular world.

We perceive the benefits from allowing students to build their own models of the molecular world as threefold. First, constructing a model allows students to concretize their understanding with a visual representation that provides them with an opportunity to reflect on their own learning as they build. The embedded features of a tool can help guide the student to such reflections; for instance, eChem highlights the number of bonds that are possible for individual atoms when students construct molecules, which supports learning about the concept of molecular hybridization and three-dimensional structure. Second, visualization tools provide immediate visual feedback to the student about the viability of the models that they construct. In this way, students have the opportunity to evaluate what they are building and compare it with other concepts learned in the classroom. The Connected Chemistry modeling environment achieves this by offering students the opportunity to simulate chemical interactions. If a student constructs a model in which the collision of an acid molecule and a base molecule raises the pH of a solution, a pH monitor in the visualization tool can warn students that the model's behavior violates accepted concepts of pH. Finally, constructed models can provide feedback to both the teacher and the entire classroom about one student's understanding. By viewing the model that a student constructs with a visualization tool, the instructor has a tangible measure of the student's progress to more effectively provide critical support and guidance. In much the same way, the entire class can view individual student work to share ideas and learn from each other about alternative perspectives about an idea or concept.

We advocate that novel visualization tools should be based on the theoretical tenets of constructivism and constructionism. Such environments allow students the widest range of opportunities to learn scientific concepts based on direct experience with visualization tools. This is not to say that the tools should not be used in any other manner. We believe that instructors can also employ them as effective visual aids when necessary, but such practices do not take full advantage of the capabilities of these novel tools. Activities in which students are able to build their own models of imperceptible objects adhere closest to the tenets of this principle. New tools should be embedded in curricula that allow great flexibility and interactivity beyond that of simple animations aimed at direct instruction. In the next section, we provide an example of one such novel curriculum, the Kinemage Authorship Project, that employs a constructivist pedagogy and adheres to both our design and cognitive principles.

THE KINEMAGE AUTHORSHIP PROJECT: TEACHING AND LEARNING WITH THREE-DIMENSIONAL REPRESENTATIONS

Teaching students to build ball-and-stick models allows students to not only manipulate and visualize the molecular models, but to build a new structure from a simple chemical formula. In this way, the student must provide the extra information needed to place the atoms in proper orientation. Building such a model is like thinking aloud. It is an expressive way to construct a mental model. Such a constructionist approach promotes deep understanding and forces the student to work through misconceptions that can arise with a simple lecture or textbook illustration. Indeed, individual construction projects do not have the time pressure of lecture where a brief look at a model can be misleading and students can adjust memory of the image to fit their preconceptions or generate new misconceptions.

Today, most chemists and biochemists work with more complex structures than students mighty typically see in introductory courses. Because physical models are limited in their ability to portray such structures, advanced research scientists in these domains have become dependent on computer graphics modeling programs to aid in the visualization of macromolecules. In fact, there tremendous progress over the last ten years in the development and implementation of these programs, which continue to become more widespread for research and industrial applications as well as publication (Voith, 2003). In the classroom, however, these tools have not yet enjoyed such versatility. Instructors still rely on textbooks to show illustrations captured from the programs and student interaction is often limited to a brief tutorial that uses pre-constructed renderings of molecules or molecular interactions.

In the Kinemage Authorship Project, we have developed a pedagogy for teaching with molecular graphics that follows the constructionist approach mentioned above that makes molecular modeling a more central component of the curriculum. In our courses, students choose a particular macromolecule to research and write a "molecular story" about the structure and function of that molecule. Each story includes a series of interactive graphic images along with extensive annotation via a hyperlinked text window. The student authors deliberately construct the graphic images to illustrate concepts and features of importance. The intent is to use a variety of approaches such as alternate renderings of the same structures and simple animation between alternate conformations to illustrate molecular motion to convey multilayered information embedded in the macromolecule. Overall, our guiding philosophy of the approach is to remove the clutter by taking away the "irrelevant" features of each image so that the student's attention is drawn to the subject of interest (Richardson & Richardson, 1994, 2002; White, Kim, Sherman, & Weber, 2002). This disembedding of information from a complex structure allows the student to focus on one thing at a time to promote learning and problem solving.

Because the graphic images are completely interactive, even editable, an author's original story can be changed at any time over the course of the project. New features can be added or original features can be altered or removed altogether. The entire project is saved as a plain text file called a *kinemage*, which is generated using the menu-based utility PREKIN and viewed using the program MAGE or its progeny program KING. The kinemage, then, is deliberately designed to be a means of communication of three dimensional concepts (four dimensional when one includes animation of motion). A kinemage can be likened to a children's museum where the displays are labeled, annotated, and interactive. In our curriculum, however, the students are the designers of each displayed kinemage. As much as children enjoy and learn from these museums, how much more could they learn if they actually helped construct the museum displays?

The kinemage format was chosen for this project because kinemages were originally developed as an electronic accompaniment for the journal *Protein Science* (Richardson & Richardson, 1992). Journal authors publishing a structure-based article could include a kinemage which would convey in three dimensions what the article described in two dimensions. The kinemage format was unique when developed because other authoring tools that used molecular graphics programs were not designed in this manner. Although other such programs, such as Rasmol and DeepView, contain scripting capability, they do not have the capability to annotate the scripted image through text windows, caption windows, and graphic labels. This multilayered annotation provides a direct linkage between the spatial and verbal information conveyed to the viewer. In addition to the inherent communication capabilities of the kinemage, the graphics also have features not found in the other graphic programs such as excellent depth cueing, simulation of molecular motion through animation between alternate conformations, and the ability to move features independently in order to dock or overlay features. Each of these features was designed so that the viewer might use the kinemage to support the visualization of the relevant structures instead of relying solely on an imagined mental image.

Kinemage construction is time consuming and is best done as an out-of-class assignment stretched over the course of a semester. Of course, teachers must embed such a construction project within the overall curriculum so that students can work up to it and so that it makes sense in the context of the discipline. Students must be able to draw connections between the individual project and what they are learning in lectures where instructors models the use of these three-dimensional images with both visual images and verbal explanations. This is an opportunity for the instructor to correlate the graphic images with physical models as well as both words and images from the textbook. Lecture is also an opportunity for students to see alternate renderings of a molecule (ball and stick, backbone, ribbon, spacefilling, etc.) and understand that these are images of the same molecule. As with the construction project, it is important to keep images used in lecture simple so that students are not confused by too much complexity, too soon.

In addition to introducing the students to the graphic images in lecture, it is important to also introduce them to the software and point out some of the features they will want to learn to move forward in their construction project. These include basic manipulation such as rotation, zooming, atom identification, and distance measurements. The use of motion is important to emphasize the illusion of three dimensionality of the graphic image. Motion, particularly a gentle rocking motion, is an effective way for even people without effective stereo vision to see the three dimensional aspects of a structure.

Today's students are quite experienced with observing complex, multidimensional computer graphics in computer and video games. This does not mean, however, that they see the same things that the instructor sees when they look at the projected image. An important part of using graphic images in lecture, then, is both to ask the students what they see and to draw the student's attention to visible features by asking questions to make them look more carefully at the image. The particular benefits of the visual display apply not only to student-teacher interactions but also to student-student interactions. For example, two students, John and Jane, may initially believe that there are no similarities between a protein:DNA complex that John constructed and a protein:protein complex constructed by Jane. However, when the instructor gives John and Jane the opportunity to examine the graphics annotations of each other's kinemage, they are able to put the verbal and spatial cues together to discover the common strategies nature uses to form interactions within and between molecules. Proper annotation of the kinemage associates the verbal information in the label with the spatial information in the visualization to generate a more complete understanding for both students.

In addition to exposure to kinemages in lecture, students must manipulate kinemages as part of their homework during the first half of the semester. These guided inquiry homework assignments are designed to become progressively more demanding as students gain both content knowledge and familiarity with the software. For example, students may be asked very simple questions about a kinemage at the beginning, then later be asked to generate a Ramachandran plot by measuring dihedral angles along pieces of a protein, and still later they may be asked to find charge interactions between a protein and a piece of DNA. Most standard biochemistry courses would stop at this point and assume that manipulation and interaction with molecular images assures a sufficient level of familiarity with the concepts of macromolecular structure.

To achieve a deeper level of understanding, we have students go the next step and ask them to make changes in an image and analyze the result. An example of this is found in the kinemage construction tutorial originally written by Jane and David Richardson (1994). The tutorial focuses on the construction of a variety of renderings of the caster bean biotoxin ricin. The active site of ricin contains the amino acid glutamate, which is critical for the toxicity of this poisonous protein. However, mutants of ricin which contain a different amino acid in this position are still active. Students must find out how the mutant biotoxin can remain active by using the graphic image to show how nearby glutamates can rotate into the same position as the mutated glutamate and “rescue” the activity of the toxin. To accomplish this, students must be able to visualize the 3D spatial arrangement of all of the amino acid sidechains in the vicinity as well as have a prior knowledge of the chemistry of the various functional groups on each of these sidechains. The kinemage assists students in applying their fundamental knowledge of protein sidechains by providing the external visualization of the protein so that students have more than their own mental images of the structure to rely on.

After completing the homework assignments, the software tutorial, and a literature search on their chosen topic, students then begin the actual construction of their kinemage. This requires a series of decisions about what to show and how to show it. These decisions force the student to construct an initial mental model of the molecule before they can begin construction on the graphic model. The process of construction requires an ongoing refinement of both mental and graphic models. Because the students are working with experimentally determined coordinate files as their source of molecular data, the data is in front of them and there is little room for “getting it wrong”. Students are encouraged to incorporate “new” features into their kinemages. For instance, students can show or propose things that the original scientist that solved the structure failed to consider (or at least report). This experience of constructing and annotating a series of molecular images requires much more of the student in terms of time, mental effort, and initiative than the manipulation and exploration of a preconstructed image. Consequently, we expect the mental model generated by kinemage construction to be more detailed, accurate, and long lasting than one generated from guided exploration of a preconstructed molecular structure.

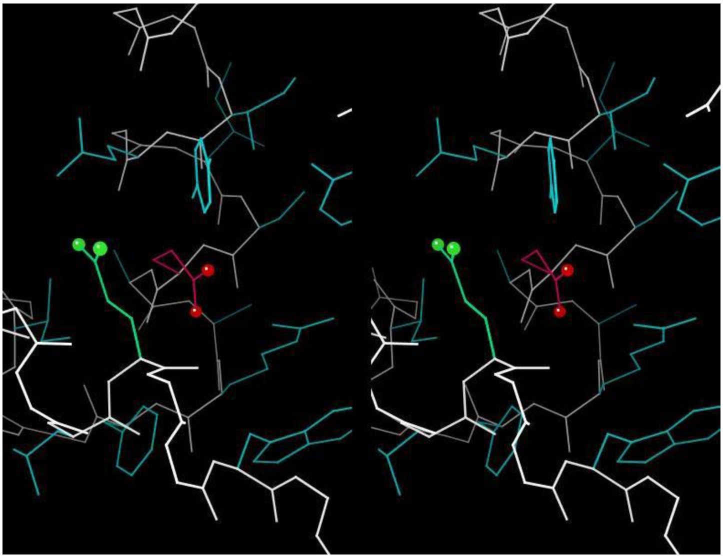

Figure 8. *Stereo kinemage of the active site of ricin showing the critical glutamate (red) and the nearby "rescue" glutamate (green). (A colour version of this diagram is included in the Colour Section)*

Our attitude assessments using surveys and interviews show that the students themselves believe this is the case (Bateman, Booth, Sirochman, Richardson, & Richardson, 2002) and anecdotal evidence long after the semester ends suggests a long lasting effect of this form of learning. For example, student authors believe they have learned more about all levels of protein structure, particularly "higher order" structure, than the control group. The more motivated students in the class particularly liked the project because it provided them an open-ended opportunity to explore as much as they like. Interestingly, we have seen no evidence of gender differences in either the quantitative or qualitative assessments despite the long-standing assumption regarding individual differences in visualization and science achievement. This is not surprising since the construction project provides lengthy training and prior studies (Roberts & Bell, 2000; Scali, Brownlow, & Hicks, 2000) have shown that gender differences in spatial ability are largely due to experience and that training can eliminate gender bias. Our project facilitates long-term experience because it extends beyond a unit or lesson as a self-paced, out-of-class assignment.

To be honest, our qualitative interviews with students have uncovered some student complaints about the kinemage construction project. The project is obviously is very time consuming and some students felt that time spent on the project took away from course fundamentals. Other students complained that the project required learning new, unfamiliar software and that this was asking too much of students. Another complaint was that the project was too focused and that students had trouble generalizing or transferring the knowledge gained about their topic to a new molecular structure. This problem of transference can be addressed in the lecture where the instructor explains connections between one image and another. This responses from students are not surprising as they are common perceptions shared by science instructors who attempt to adopt novel visualization tools (Butler & Sellbom, 2002). As we continue with our iterative development of the curricula, we hope to overcome these criticisms and maximize the positive feedback from students.

CONCLUSION

Throughout this chapter we have advocated for the use of visualization tools in the science classroom. Visualization tools are now available to aid students in the visualization of raw data, abstract concepts, and imperceptible entities. We believe that these tools hold much promise for the teaching and learning of science by providing virtual three-dimensional representations of such objects, events, and phenomena, which are often directly imperceptible to students. Although most current claims regarding the effectiveness of these tools remain based on anecdotal evidence, we believe that more substantiated claims are forthcoming. We consider one fruitful path to such claims to lie in collaborations between designers of visualization tools, science instructors, and cognitive scientists. At present, we suggest that such collaborations should aim to develop strong theoretical frameworks that motivate and explicate the role of visualization tools in the science classroom and the use of visualization as a cognitive strategy in science learning and problem solving.

To that end, we have offered an initial theoretical framework that combines cognitive theories of visualization with constructivist and constructionist theories of pedagogy. Our framework posits three principles for the design and implementation of visualization software in the sciences, particularly chemistry. Our first principle stipulates that visualization tools should be designed to support spatial cognition in learning and problem solving. The general goal that visualization tools allow students to appreciate imperceptible entities is insufficient to achieve significant learning gains. Instead, we believe it is more productive to identify the specific manner in which a visualization tool assist students both to perceive complicated or imperceptible three-dimensional relationships and to generate more accurate mental representations of concepts and phenomena.

Second, we suggest that a strong cognitive model of the role of visualization in science learning and problem solving is needed to specify and assess the role of visualization tools in students' learning. Too many designs have been motivated by the assumption that visualization is important simply because science domains often deal with three-dimensional objects interacting in an imperceptible three-dimensional space. We consider visualization to be an essential and task-specific cognitive strategy in science based on research from cognitive science regarding the encoding and manipulation of spatial information. That research has shown that individuals can perceive and encode spatial information in multiple modalities as a function of the form in which that information is displayed. Moreover, similar lines of research in science education community have indicated that students can alternate between the use of visualization strategies and non-imagistic heuristics as their experience grows. We suggest that productive research agendas lie in investigating the interaction between these two strategies and how visualization tools may mediate that interaction.

Finally, we believe that students and teachers stand to gain the most positive learning outcomes from implementing visualization strategies according to constructivist and constructionist philosophies of learning and teaching. That is, visualization tools are least effective when implemented as a supplemental aid to traditional lessons in the science classroom. A more productive use of these tools is achieved when they become a central feature of novel pedagogies. According to these philosophies students benefit the most from opportunities to build their own visual representations of domain concepts and phenomena in activities like those in the Kinemage Authorship Project. Activities such as these provide students and teachers with direct visual feedback on learning and understanding and they promote recursive self-reflection and collaboration among students.

The three principles of our theoretical framework present unique questions for the science education community to probe. For example, clarifying the role of visualization as a cognitive strategy in science problem solving suggests new agendas to the study of learning and performance. Although previous research agendas have focused specifically on determining the impact of individual differences in visuo-spatial ability in science learning, our framework suggests that more pointed questions are necessary. At the least, we must ask when and how students employ visualization with both traditional problems and with the use of visualization tools. Such an investigation moves beyond determining simple correlations and asks whether visualization tools support poor visuo-spatial abilities or illicit unique problem solving strategies that obviate visualization altogether. Consequently, the findings from such studies can implicate new methods for assessing the impact of visualization tools on learning. By first targeting the role of visualization strategies during problem solving, we can begin to clarify the contradictory evidence for learning gains produced to date.

More broadly, as the effectiveness of using visualization tools in the science classrooms is revealed, we can begin to ask fundamental questions about the implications such tools have for future science curricula. Currently, most instructors employ visualization tools sporadically in curricula that remain mostly traditional in nature. Alternatively, the Kinemage Authorship Project provides one example in which the visualization tool significantly alters the type of learning in which students engage. Instead of simply using the tool as a visual aid, students use kinemages to conduct research investigations by constructing models of proteins and enzymes to probe function. If the end result of such an implementation proves to instill deeper conceptual knowledge and active engagement, the continued use of traditional modes of instruction must be scrutinized. As visualization tools are optimized through iterative development and strong theoretical frameworks emerge to situate the role of these tools in scientific cognition, new models of science curricula must adapt to take advantage of them. These changes will be facilitated by the kinds of interdisciplinary collaborations between chemists, cognitive scientists, and educators that are a characteristic of the chapters in this volume.

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AUTHOR NOTE

Color versions of all figures included in this chapter are given in the accompanying CD-ROM.