Molecular visualization in chemistry education: the role of multidisciplinary collaboration

Loretta L. Jones*,[1] Kenneth D. Jordan[2] and Neil A. Stillings[3]

[1] University of Northern Colorado, Department of Chemistry and Biochemistry, Greeley, CO, USA.
email: Loretta.jones@unco.edu
[2] University of Pittsburgh, Department of Chemistry and Center for Molecular and Materials Simulations, Pittsburgh, PA, USA.
email: Jordan@psc.edu
[3] School of Cognitive Science, Hampshire College, Amherst, MA, USA.
email: nstillings@hampshire.edu

Received 11 March 2005, accepted 2 June 2005

Abstract: Visualization tools and high performance computing have changed the nature of chemistry research and have the promise to transform chemistry instruction. However, the images central to chemistry research can pose difficulties for beginning chemistry students. In order for molecular visualization tools to be useful in education, students must be able to interpret the images they produce. Cognitive scientists can provide valuable insight into how novices perceive and ascribe meaning to molecular visualizations. Further insights from educators, computer scientists and developers, and graphic artists are important for chemistry educators who want to help students learn with molecular visualizations. A diverse group of scientists, educators, developers, and cognitive psychologists have begun a series of international collaborations to address this issue. The effort was initiated at the National Science Foundation supported Molecular Visualization in Science Education Workshop held in 2001 and has continued through a series of mini-grants. These groups are investigating characteristics of molecular representations and visualizations that enhance learning, interactions with molecular visualizations that best help students learn about molecular structure and dynamics, roles of molecular modeling in chemistry instruction, and fruitful directions for research on molecular visualization in the learning of chemistry. This article summarizes the value of collaboration identified by participants in the workshop and subsequent collaborations. [*Chem. Educ. Res. Pract.*, 2005, **6** (3), 136-149]

Keywords: molecular visualization; modeling; particulate nature of matter; computer-assisted education; collaboration; multidisciplinary.

> *Do not underestimate the power of kinetic art…Pictures seldom can capture all the subtle nuances of a model, but good pictures and movie clips are not only what are best remembered, they also often enable us to take the next steps in both teaching and research.* (Zare, 2002)

The importance of collaboration

Chemistry research today is increasingly focused on phenomena that are understood and communicated by means of visual representations. For example, research on carbon nanotubes, conducting polymers, drug design, and self-assembling materials is carried out and communicated with the help of computer-generated images. Some chemical phenomena are not obvious without the use of visualizations; visualization tools such as molecular modeling programs are required to describe and study them. Using these tools requires the ability to identify and make use of complex visualizations of molecular structures. However, technologies developed for molecular research generally involve interfaces that were optimized for research purposes and may be difficult for beginners to use (Edelson and Gordin, 1997). Fluency with molecular visualization tools is becoming a literacy requirement for chemists, but new interfaces may be required in order for molecular visualization tools to be successful in education.

Visualization tools are now beginning to be used in a central way in the introductory chemistry classroom (Jones, 2001; Tasker, 2004). Beginning chemistry students can now be exposed to a wide array of molecular visualizations: structural formulas, line drawings, physical models, a variety of dynamic three-dimensional computer-generated molecular models, and images generated by instruments such as scanning tunneling microscopes. Learning from these molecular visualizations is challenging for students because they can be complex and require a variety of skills to interpret (Kozma and Russell, 1999). However, the understanding and use of a variety of molecular representations is important in understanding the particulate nature of matter (Griffiths and Preston, 1992; Johnstone, 1993; Bodner and Domin, 2000). The merging of scientific fields with disciplines such as art, psychology, and technology can result in visualizations that are not only effective in communicating concepts, but are also easily interpreted by beginning students (Gordin and Pea, 1995). These interdisciplinary collaborations are important for visualizations of the particulate level of matter to be effective learning tools.

The knowledge and skills required to produce pedagogically effective visualizations and to apply them appropriately for learning go beyond the knowledge of chemistry to encompass the findings of cognitive science and the principles of pedagogy. The need to apply knowledge from multiple disciplines toward the improvement of chemistry education has been recognized by others (Bailey and Garratt, 2002; Bucat, 2004; Gilbert et al., 2004). This paper describes a rationale and model for real-time collaborations between chemists, educators, and cognitive psychologists to develop visualizations, to design effective pedagogical uses of visualizations, and to conduct research studies of learning from visualizations.

In 2001 the United States National Science Foundation supported a project to build collaborations among diverse research communities in order to investigate molecular visualization in the teaching of chemistry. The initial activity of the project was the Molecular Visualization and Science Education Workshop held in Arlington, Virginia, USA, which was organized by the authors of this paper. Thirty-six scientists, developers, cognitive psychologists, and science educators met to examine characteristics of molecular representations, interactions with visualizations of molecular structure and dynamics, the role of molecular modeling in chemistry curricula, and fruitful directions for research on molecular visualization in the learning of chemistry.

The workshop explored the frontier between the physical and cognitive sciences. In particular, the participants examined how research findings from the cognitive sciences can be applied to improve chemical education as well as the design of visualization tools. All types of molecular models were considered, including physical models. However, computer-based multimedia and molecular modeling tools became the primary focus of the workshop, because of their potential to make a profound difference in how molecular-level concepts are learned (Williamson and Abraham, 1995; Hehre and Nelson, 1997; Shusterman and Shusterman, 1997; Smith, 1998; Jones, 1999; Dori and Barak, 2001).

Workshop participants readily saw that each discipline had a separate, but essential role to play in the development and use of molecular visualizations in the learning of chemistry. It soon became apparent that multidisciplinary collaborations would enable projects more ambitious than participants might otherwise have considered. An independent evaluation of the workshop conducted by José and Williamson (2005) found that immediately following the workshop 72% of the participants agreed with the statement, "*The interdisciplinary interactions at this workshop have encouraged me to work with others outside my own perspective on projects*." That this effect was fundamental and lasting is suggested by the fact that after one year had passed, 76% agreed with the statement. The workshop report, which summarizes the discussions, is available on-line (Jones et al., 2001).

The next phase of the project was the funding of six small projects called mini-grants to promote collaboration across the disciplines of science, cognition, and education in support of visualization in science education (Jones, 2004; also see the Appendix at the end of this paper). These collaborations, which involve investigators from seven disciplines and seven nations, have begun to address the issues raised at the workshop by initiating pilot research studies and by developing a variety of instructional materials.

This article reports on the potential benefits of interdisciplinary collaboration for molecular visualization that were identified in the workshop and how they have been developed through subsequent collaborations. It also outlines guidelines for such collaborations that have proved beneficial.

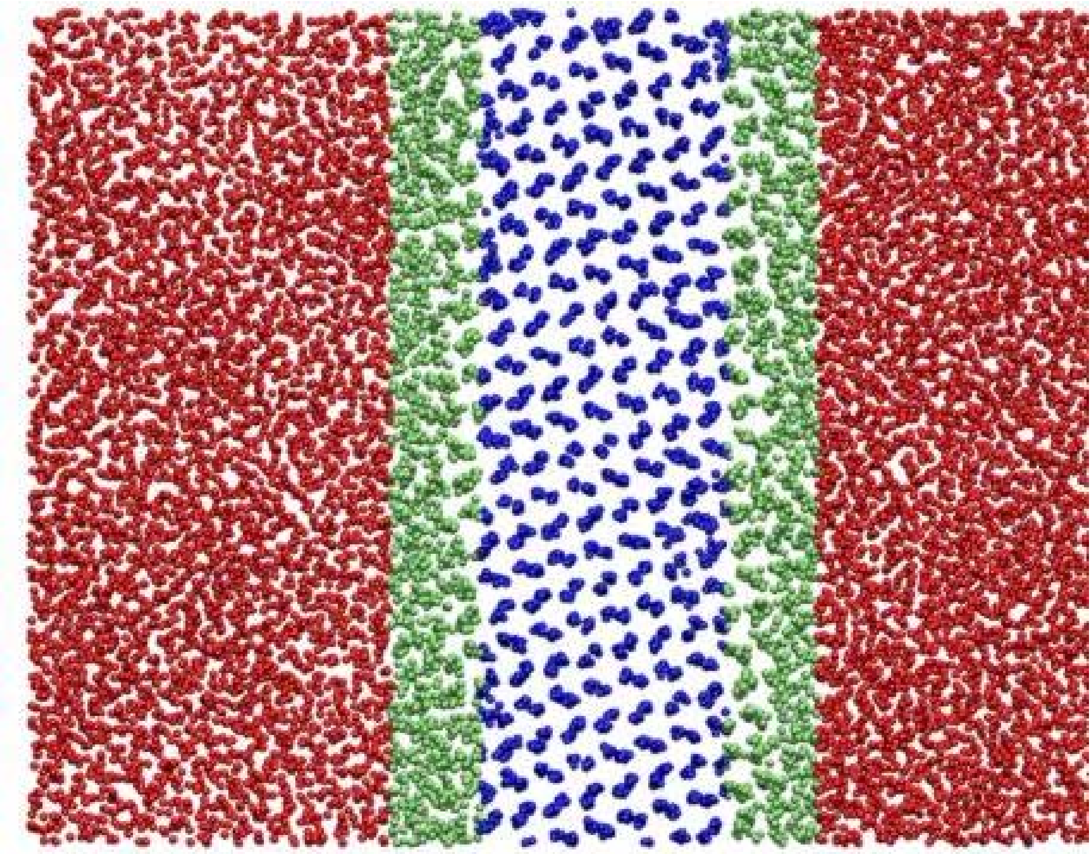
A cognitive science perspective on learning from molecular visualizations

In the past the term *visualization* was used to refer simply to the process of imagining, but the term is now being applied to images that enhance our imagination and visual experience. Visualizations can extend the visual memory and thinking processes of chemists by providing dynamic images of virtual worlds (Shepard and Cooper, 1982). These images are used to convey complex, subtle molecular interactions and dynamics that are difficult to describe in words. For example, they can show chemists the flexibility of proteins, the mechanism by which ions pass through membrane channels, and how heating a molecule affects its reactivity.

A chemist can 'see' the theory underlying a visualization. However, cognitive scientists have shown that the visual system has limited neural resources (Trick and Pylyshyn, 1994). Therefore, visualizations of abstract molecular concepts may be too complex for learners to process. For students to learn from an image, they must attend to its relevant characteristics and understand how they demonstrate new concepts. They must also know the scientific conventions (Habraken, 1996) and learn to tune out irrelevant or distracting information (Kozma and Russell, 1997). For example, Figure 1 was produced for use in research on the structure of water by a molecular dynamics NAMD simulation (Humphrey et al., 1996; Kalé et al., 1999). A chemist involved in this research will see in the image how the structure of water changes when ice melts, but without guidance a beginning student—even a chemist not familiar with the representational conventions—may see only a confusing array of molecules.

Cognitive scientists participating in the workshop and collaborations described in this paper reported that the difficulties students face in understanding and using molecular visualizations can tentatively be divided into four areas: visual subtlety, complexity, abstractness, and conceptual depth (Jones et al., 2001). These difficulties may not be apparent to chemists who are fluent users of visualizations. However, they pose important research and design challenges for chemistry instructors and for developers of molecular visualizations.

Figure 1.



What do you see in this picture? The image is a ‘snapshot’ from a 500 ps molecular dynamics NAMD simulation that shows how the structure of water changes when ice melts. The red spheres represent liquid water molecules, blue spheres represent ice, and green spheres represent water in the interfacial region. The image shows researchers that water molecules form clusters when they melt (the clusters can be seen in the interfacial region). Image provided by Jeffry Madura with the assistance of Pranav Dalal (Center for Computational Sciences), Duquesne University.

Visual subtlety: Spatial relationships in molecular visualizations can be difficult to interpret. Some examples are the two-dimensional display of three-dimensional structures, the fact that a variety of angles other than 90° occur in molecular structures, and the need simultaneously to track the motion or arrangements of multiple objects.

Complexity: Interpreting a molecular structure may be a complex process when the amount and depth of information encoded in the representation is large and when different representations must be used and compared. Although students benefit when different types of representations are used to convey different conceptual content, learning to understand each variety of representation and the interrelations among them is a complex process.

Abstractness and conceptual depth: Molecular visualizations use a set of conventions to represent phenomena not normally visible. The conventions are readily understood by chemists, but beginning students must learn to interpret these conventions. In ball-and-stick molecular models, for example, the balls and sticks are symbols that stand for things that have few of the properties of the symbols themselves. Students must learn to make connections between molecular representations (the balls and sticks) and the concepts they represent (atoms and chemical bonds).

Expert chemists can link theory and appearance to ‘see’ the theory in a molecular structure. For novice learners the relationship between a visualization and the underlying concepts is much more difficult to understand. In order to learn more about a concept from a visualization they must already have some knowledge about the concept and how it is represented by the visualization (Treagust et al., 2003). The visual subtlety, complexity, and conceptual depth of molecular visualizations present important research and design challenges to chemistry instructors, curriculum developers, and educational researchers.

The place of molecular visualization in the curriculum

Mathematics curricula based on multiple representations have been found to provide teachers with a greater variety of instructional and assessment approaches than do traditional curricula (Cuoco and Curcio, 2001). Similar findings have also been reported in chemistry classrooms (Russell et al., 1997). Participants in the collaborations described here devised a set of characteristics that should be considered when introducing molecular visualizations into the tertiary general chemistry curriculum (Jones et al., 2001). These include providing opportunities for practice and feedback on learning, appropriate annotation of visualizations, gradual introduction of conventions and structural complexity, comparative presentation of related visualizations, the use of animations, provisions for appropriate interactions with the visualizations, and instructional materials designed for concept mastery and inquiry.

Interactive computer-generated molecular visualizations provide many opportunities for instructional innovation. They are being used not only to encourage students to think about chemistry in terms of molecules, models, and symbols, but also to provide opportunities for students to become more independent learners (Agapova et al., 2002). In addition, interactive visualizations can help instructors interest and motivate students with a variety of learning styles (Suits, 2003). To achieve these goals, more activities incorporating visualizations that are easy for students to use and interpret will need to be developed.

Many topics in chemistry require learners to understand structures in three dimensions, changes over time, and causality. Molecular animations can be powerful tools for learning these dynamic and three-dimensional chemistry concepts (Tasker, 2004). However, a problem with the use of animations for teaching molecular structure and dynamics is that merely viewing a visualization may lead to learning at a lower level than would drawing or building a molecular structure. Consequently, it may be beneficial for computer-based visualizations to provide opportunities for students actively to explore concepts (Khan, 2001).

At the high end of technological development are novel learning environments that help students to visualize complex or invisible phenomena through immersion in a virtual reality (Johnson et al., 2001). Virtual reality offers the potential for exploring complex molecular structures from many vantage points, even from the inside out. However, the more complex the representations the more guidance and scaffolding is required for students to interpret them (Suits and Diack, 2002; Ardac and Akaygun, 2004; Kuo et al., 2004).

Research on molecular visualizations in chemical education

Because molecular visualization plays a central role in much chemistry and biology research, research into the characteristics and modes of interaction with visualizations used by scientists is as important as research into learning with visualizations. Although some work is currently being conducted in these areas, our knowledge of how visualizations can best be created and used is still tentative. Interdisciplinary collaborations involving chemists, biologists, cognitive scientists, and science educators may enhance these research studies.

Research on characteristics of molecular visualizations can address such questions as, "*What are the effects of visualizations on intuitions, research questions, conceptions, and misconceptions?*" and "*What principles of graphic design are important for the design of effective molecular visualizations*?" Research on modes of interaction with visualizations can address questions such as, "*How do student mental models of matter change as a function of interaction with molecular visualizations*?" and "*Which learning method is most appropriate for a given learning situation?*" Research on curriculum issues is needed to study issues such as the problem-solving skills required for interpreting different kinds of visualizations, how the curriculum can be restructured to incorporate visualizations, the extent of guidance students need to interpret specific types of visualizations, and how learning from visualizations can best be assessed.

Building fruitful collaborations between disciplines

At the 2001 Gordon Research Conference on Visualization in Science and Education the US National Science Foundation solicited and funded six small projects called mini-grants to promote collaboration across the disciplines of science, cognition, and education in support of visualization in science education (see the Appendix at the end of this paper). Each project received US$5000 to facilitate interdisciplinary and multidisciplinary collaboration. These collaborations, which involve participants representing thirteen disciplines, have begun to address the issues raised at the workshop by conducting pilot research studies and by developing a variety of instructional materials. A second round of five mini-grants, administered by Mary Jane Shultz, Tufts University, were awarded in 2003. The Appendix at the end of this article contains a brief description and contact information for each of the six completed projects.

Outcomes of the mini-grant program

The outcomes of the mini-grant projects far exceeded expectations. The participants reported that they had carried out projects not otherwise possible without the multidisciplinary collaborations, had initiated additional collaborative research and development efforts, and had identified barriers to collaboration between disciplines for work in this area. The six collaborations involved participants from more than twenty-five institutions and seven nations. Research studies on learning from visualizations were conducted in nine of the institutions. Twenty conference presentations reported the results of these projects, two articles have been published (Dori et al., 2003; Velázquez-Marcano et al., 2004), and several articles are in preparation.

A variety of products were produced in the collaborations, including new evaluation instruments, websites for research or dissemination, digital videos of chemical demonstrations and experiments, a set of animations, instructional software programs, paper instructional materials, and two annotated bibliographies.

Three major obstacles were encountered by the mini-grant teams. One was the need to overcome different views on project goals and activities that often arose from differences in disciplines and types of institutions. The second was the need to frame projects in such a way that they would be acceptable for promotion of participants within science departments. Some promotion and tenure committees did not understand how to evaluate the work being done. The third was the difficulty of maintaining frequent communication among participants at geographically distant institutions. Minor problems reported included the difficulty in finding times when all the collaborators were available to meet, coping with the time required for the work, and changes in personnel.

Many benefits of the collaborations were cited by project participants, including new ties across disciplines, the development of new instructional tools, research instruments, and protocols, and the new perspectives gained from other disciplines. The participants felt that the collaboration between disciplines was a strength of their projects and they reported that they would not have been able to tackle the projects alone. The scientists felt that they had gained the ability to set appropriate learning objectives, had developed a greater awareness of student learning needs, an appreciation of the difficulties of evaluating major instructional change, the ability to design assessment tools, and the confidence to tackle complex projects that require expertise in other disciplines. One investigator, Peter Mahaffy, reported the following (Lewis and Mahaffy, 2003):

> "*In my experience, the most valuable dimension to the mini-grant was the way it formalised working across learning communities. Natural scientists with experience in visualization, social scientists, teachers, and curriculum planners all engaged in conversation and testing to learn how visualizations are culturally laden. In the process of trying to understand the cultural dimensions to visualization, we have also carefully identified some more fundamental questions about what constitutes an effective visualization.*"

Recipients of the mini-grants reported that they would not have been able to carry out the interdisciplinary projects without the stimulus of the mini-grant funds. Although the dollar amount was very small, it was enough to bring together individuals with complementary expertise. The majority of the mini-grant participants reported that they plan to continue their work in the area of scientific visualization in education.

The mini-grant recipients reported a number of factors that they felt led to successful collaborations. These factors include common goals, mutual interests in the educational applications of scientific visualizations, additional funds from other sources, pre-existing connections among the participants and with other, related projects, proximity of the participants to one another, and supportive colleagues and institutions. The following case study illustrates how the efforts of one mini-grant team managed to overcome difficulties and achieve a synergy beyond that which team members could have managed individually.

Testbeds for new visualizations in organic chemistry: Case study of a mini-grant

One of the authors of this paper, Neil Stillings, was the Co-Principal Investigator of a mini-grant project. The work was carried out under the leadership of Carl Wamser, a chemist at Portland State University (PSU) in Oregon, on the West Coast of the U.S., while Stillings, a cognitive psychologist, is based on the East Coast, 3000 km and three time zones away. Locations of the additional participants and consultants, Pratibha Varma-Nelson (Northeastern Illinois University), Jack Kampmeier (University of Rochester), Don Wedegaertner (University of the Pacific), and Gwen Shusterman (Portland State University), were equally widespread.

The majority of the work was performed at Portland State University, where the subject students were enrolled, and where the two Principal Investigators met to administer the new tests and surveys. The project was carried out in an organic chemistry course in which an innovative teaching environment, Peer-Led Team Learning workshops, had been introduced (http://www.sci.ccny.cuny.edu/~chemwksp/). The goal of the project was to create new visualization exercises and assessments of stereochemistry that could be used within this workshop learning environment and would also be valuable in traditional classrooms. Wamser would develop the exercises and Stillings the assessments.

Stillings felt that he needed to know more about the chemistry before he could begin. Therefore, one of his first activities was to visit PSU, where he attended organic chemistry classes and workshop sessions as an unobtrusive observer. He studied how the students used molecular models and 3D computer visualizations to develop an understanding of stereoisomerism. He also obtained a model kit and an organic chemistry textbook in order to learn the stereochemistry concepts taught in the course. This initial background work allowed him to create a specialized organic chemistry analog of a commonly used generic mental rotation test (Peters et al., 1995).

The new test was administered to students along with a questionnaire that asked the students to characterize their mental rotation strategies and to reflect on the ways in which three-dimensionality can be perceived and manipulated. Preliminary results show that students significantly improved their scores after participating in peer-led workshops in which they were required to build three-dimensional models to illustrate stereochemistry concepts.

The team kept in touch through frequent email exchanges and conference calls. They felt that maintaining frequent contact allowed the development of the testing and assessment methods to proceed smoothly despite the distance and the different disciplinary backgrounds. They also felt that the work would not have been possible without the collaboration fostered by the mini-grant (Wamser and Stillings, 2003):

> "*This work would not have happened without the stimulus of the NSF mini-grant. The specific manner in which it was carried out could not have happened without the blending of the two unique approaches brought by the two PIs. Each of us has become much more aware of the other's field of study and the potential for interrelationships between the fields. In particular, neither of us would have had the expertise or confidence to have tackled an interdisciplinary project like this alone*."

Summary

The workshop and projects described in this paper show that the field of molecular visualization can benefit from collaborations that involve chemists, educators, cognitive psychologists, and other professionals. The workshop, which brought together multiple disciplines with a common agenda, was found to be instrumental in promoting these collaborations. José and Williamson reported in an evaluation of the workshop (2005) that the workshop "*made progress toward defining the role/nature of molecular visualization in science education*," served as a model of successful interdisciplinary collaboration, and acted as a catalyst for research into learning from molecular visualization. The workshop also served to raise awareness within the cognitive science community of molecular visualization as a research area. This multidisciplinary workshop model has now been successfully applied in geoscience education (Manduca et al., 2004).

Participants in the Workshop for Molecular Visualization in Science Education found that communication between disciplines is not only important between educational researchers and classroom teachers (de Jong, 2000), it is necessary between educational researchers and chemists, psychologists, and professionals from other fields. Collaborations involving chemists, cognitive scientists, science educators, and others are needed to carry out research studies on learning with molecular visualizations. The success of the mini-grant program suggests that small multidisciplinary projects that promote collaboration on such research efforts may be successful.

Individuals wanting to become involved in multidisciplinary collaborations in molecular visualization can find willing collaborators at conferences such as the Gordon Research Conference on Visualization in Science and Education, which is currently scheduled in odd-numbered years in Oxford, England. Information on this conference series is available at http://www.grc.org/programs/2005/visualiz.htm. Several other conference series promote multidisciplinary collaboration for scientific visualization in instruction. Two are the IEEE

Visualization Conference, http://vis.computer.org/, and Ed-Media, which is sponsored by the Association for the Advancement of Computing in Education, http://www.aace.org/conf/edmedia/.

Acknowledgements

The authors would like to thank Jeffry Madura, Duquesne University, for providing the figure, Joe Grabowski, University of Pittsburgh, for his helpful comments on the article, and Nora Sabelli, SRI International, for her encouragement and for helping to shape the ideas that led to this project. This material is based upon work supported by the US National Science Foundation under Grant No. 0095023.

References

Agapova O.I., Jones L.L., Ushakov A.S., Ratcliffe A.E. and Varanka Martin M.A., (2002), Encouraging independent chemistry learning through multimedia design experiences, *Chemical Education International*, **3,** AN-8. Available at: http://www.iupac.org/publications/cei/vol3/0301x0an8.html.

Ardac D. and Akaygun S., (2004), Effectiveness of multimedia-based instruction that emphasizes molecular representations on students' understanding of chemical change, *Journal of Research in Science Teaching*, **41**, 317-337.

Bailey P.D. and Garratt J., (2002), Chemical education: theory and practice, *University Chemistry Education*, **6**, 39-57.

Bodner G.M. and Domin D.S., (2000), Mental models: the role of representations in problem solving in chemistry, *University Chemistry Education*, **4**(1), 24-30.

Bucat R., (2004), Pedagogical content knowledge as a way forward: applied research in chemistry education, *Chemistry Education: Research and Practice*, **5**, 215-228.

Cuoco A.A. and Curcio F.R., (2001), *The roles of representation in school mathematics*. 2001 Yearbook, Reston, VA, National Council of Teachers of Mathematics.

de Jong, O., (2000), Crossing the borders: chemical education research and teaching practice, *University Chemistry Education*, **4**, 31-34.

Dori Y.J. and Barak M. (2001). Virtual and physical molecular modeling: fostering model perception and spatial understanding. *Educational Technology & Society*, **4**, 61-73.

Dori, Y.J., Barak M. and Adir, N., (2003), A web-based chemistry course as a means to foster freshmen learning. *Journal of Chemical Education*, **80**, 1084-1089.

Edelson, D. C. and Gordin, D. (1997) Creating science learning tools from experts' investigation tools: a design framework, *Annual Meeting of the National Association for Research in Science Teaching*, Oak Brook, IL, March 20-24, 1997.

Gilbert J.K., Justi R., Van Driel J.H., De Jong, O. and Treagust, D.F., (2004), Securing a future for chemical education, *Chemistry Education: Research and Practice*, **5**, 5-14.

Gordin D.N. and Pea R.D., (1995), Prospects for scientific visualization as an educational technology, *Journal of the Learning Sciences*, **4**, 249-279.

Griffiths A. and Preston K., (1992), Grade 12 students' misconceptions relating to fundamental characteristics of atoms and molecules, *Journal of Research in Science Teaching*, **29**, 611-628.

Habraken C., (1996), Perceptions of chemistry: why is the common perception of chemistry, the most visual of sciences, so distorted?, *Journal of Science Education and Technology*, **5**, 193-201.

Hehre W.J. and Nelson J.E., *Introducing molecular modeling into the undergraduate chemistry curriculum*, Wavefunction Inc., Irvine, CA, 1997.

Humphrey W., Dalke A. and Schulten K., (1996), VMD (Visual Molecular Dynamics), *Journal of Molecular Graphics*, **14**, 33-38.

Johnson A., Moher T., Ohlsson S. and Leigh J., (2001) Exploring multiple representations in elementary school science education. *Proceedings of IEEE Virtual Reality 2001*, March 13-17, Yokohama, Japan.

Johnstone A.H., (1993), The development of chemistry teaching: a changing response to changing demand, *Journal of Chemical Education*, **70**, 701-704.

Jones L.L., (1999), Learning Chemistry through Design and Construction, *UniServe Science News*, **14**, November, 3-7.

Jones L.L., (2004), *Molecular visualization and science education: promoting collaboration across disciplines, NSF Grant 0095023*, Unpublished report to the National Science Foundation.

Jones L., Jordan K and Stillings N., (2001), *Molecular visualization in science education*, Available at http://pro3.chem.pitt.edu/workshop/workshop_report_180701.pdf .

Jones M.B. (2001), Molecular modeling in the undergraduate chemistry curriculum, *Journal of Chemical Education*, **78**, 867-868.

José, T. and Williamson V., (2005), Molecular visualization and science education: an evaluation of the NSF-sponsored workshop *Journal of Chemical Education*, **82**, 937-943.

Kalé L., Skeel R., Bhandarkar M., Brunner R., Gursoy A., Krawetz N., Phillips J., Shinozaki A., Varadarajan K. and Schulten K., (1999), NAMD2: Greater scalability for parallel molecular dynamics, *Journal of Computational Physics,* **151**, 283-312.

Khan S., (2001), Developing inquiry skills while learning about unobservable processes in chemistry. Presented at the *American Educational Research Association Annual Meeting*, Seattle,WA, April, 2001.

Kozma R.B. and Russell J., (1997), Multimedia and understanding: expert and novice responses to different representations of chemical phenomena, *Journal of Research in Science Teaching*, **34**, 949-968.

Kuo M-T., Jones, L.L., Pulos S.M. and Hyslop R.M., (2004), The relationship of molecular representations, complexity, and orientation to the difficulty of stereochemistry problems, *The Chemical Educator,* **9**, 321-327.

Lewis N. and Mahaffy P., (2003), Final report – NSF minigrant for cross-cultural issues in building science education capacity through visualizations in chemistry and physics.

Manduca C., Mogk D. and Stillings N., (2004), *Bringing research on learning to the geosciences: report from a workshop sponsored by the National Science Foundation and the Johnson Foundation*, Available at Bridging research on learning to the geosciences workshop, Wingspread Foundation, Racine, WI, July 8-10, 2002; see http://dlesecommunityserc.carleton.edu/research_on_learning/workshop02/

Peters M., Laeng B., Latham K., Jackson M., Zaiyouna R. and Richardson C., (1995), A redrawn Vandenberg & Kuse mental rotation test: different versions and factors that affect performance, *Brain and Cognition,* **28**, 39-58.

Russell J. W., Kozma, R. B., Jones, T., Wykoff J., Marx N. and Davis, J., (1997), Use of simultaneous-synchronized macroscopic, microscopic, and symbolic representations to enhance the teaching and learning of chemical concepts, *Journal of Chemical Education*, **74**, 330-1085.

Shepard R.N. and Cooper L.A., *Mental images and their transformations*, MIT Press: Cambridge, MA, 1982.

Shusterman G.P. and Shusterman A., (1997), Teaching chemistry with electron density models, *Journal of Chemical Education*, **74**, 771-776.

Smith S.G., (1998), From mainframes to the web, *Journal of Chemical Education*, **75**, 1080-1085.

Suits J.P. and Diack M., (2002), Instructional design of scientific simulations and modeling software to support student construction of perceptual to conceptual bridges, *Educational Multimedia, Hypermedia & Telecommunications, Proceedings,* **3**, 1904-1909.

Suits J.P., (2003), Aesthetic constructivism: development of expertise in science classrooms, *National Forum of Applied Educational Research Journal*, **17**, 46-53.

Tasker R., (2004), Using multimedia to visualize the molecular world: educational theory into practice. In *A Chemist's Guide to Effective Teaching*, Pienta N., Greenbowe T. and Cooper M., eds., Chapter 16, pp. 256-272, Prentice Hall.

Treagust D.F., Chittleborough G. and Mamiala, T.L., (2003), The role of submicroscopic and symbolic representations in chemical explanations, *International Journal of Science Education*, **25**, 1353-1368.

Trick L.M. and Pylyshyn Z.W., (1994). Why are small and large numbers enumerated differently? A limited capacity preattentive stage in vision. *Psychological Review*, **100**, 80-102.

Velázquez-Marcano A., Williamson V., Ashkenazi G., Tasker R. and Williamson, K., (2004), The use of video demonstrations and particulate animation in general chemistry, *Journal of Science Education and Technology*, **13**, 315-323.

Wamser C. and Stillings N., (2003), Final report–NSF mini-grant for peer-led chemistry workshops as test beds for new visualizations in organic chemistry.

Williamson V.M. and Abraham M.R., (1995), The effects of computer animation on the particulate mental models of college chemistry students, *Journal of Research in Science Teaching*, **32**, 521-534.

Zare R., (2002), Visualizing chemistry, *Journal of Chemical Education*, **79**, 1290-1291.

Appendix: Summaries of the Mini-grant Projects

This listing includes only the Principal Investigators and Co-Principal Investigators of each project and a brief summary of the accomplishments. Many additional participants were involved and extensive additional activities were carried out. Principal Investigators can be contacted for further information on the individual projects. All participants are from the United States unless otherwise indicated.

1. Towards the general chemistry course of the year 2050

Principal Investigator: Peter Garik, Boston University
Co-Principal Investigators:
Yehudit Dori, Technion, Israel University of Technology, Haifa, Israel
Morton Hoffman, Boston University
Kenneth Jordan, University of Pittsburgh
Contact: Peter Garik, garik@bu.edu

Summary: This project was designed to set up pilot tests of new instructional approaches incorporating visualization in a small honors course at Boston University. The investigators were able to modify their goals to include the large introductory chemistry course, due to the interest of an additional faculty member at Boston University. Their final goals included the refinement of a computer-based visualization tool for learning quantum mechanics, creating an instructional unit for the tool, develop an instrument to measure the effect of the tool on students' knowledge and beliefs, and providing access to the software through a website.

2. Cross-cultural issues in building science education capacity through visualizations in chemistry and physics

Principal Investigator: Nathan Lewis, California Institute of Technology and Caltech Chemistry Animation Project
Co-Principal Investigators:
Peter Mahaffy, The King's University College, Edmonton, Alberta, Canada
Natalia Tarasova, Professor and Director, Institute for Problems of Sustainable Development, Moscow, Russia
Zafra Lerman, Columbia College, Chicago
Brian Martin, The King's University College, Edmonton, Alberta, Canada, and Alberta Modular Approach to Physics Project
Clarence Joldersma, Associate Professor of Education, Calvin College, Michigan
Leanne Willson, Psychology, University of Alberta, Canada
Contacts:
Nathan Lewis, nslewis@its.caltech.edu
Peter Mahaffy, pmahaffy@KingsU.ab.ca

Summary: This proposal provided seed funding to bring together developers of significant visualization tools in chemistry and physics with experts in cognition, education, pedagogy, assessment, and cross-cultural issues. It piloted the use of these visualization tools in a development context, thus extending discussions about visualization in science to include collaborators from Eritrea in the science of learning and the learning of science. A detailed annotated bibliography on cross-cultural issues in science education was prepared and disseminated among project participants. Project materials were evaluated then implemented in the Chemical Liceum in Khimki, Moscow region of Russia, and at several institutions in Eritrea: the Chemistry, Physics, and Education Departments of the University of Asmara, the Eritrean Ministry of Education (for a panel of curriculum leaders), and a library in Decamare.

3. Assessment strategies for instruction using molecular visualizations

Principal Investigator: Duane W. Sears, University of California-Santa Barbara
Co-Principal Investigators:
Robert C. Bateman, University of Southern Mississippi
Brian T. White, University of Massachusetts
David Uttal, Northwestern University
Contact: Duane Sears, sears@lifesci.ucsb.edu

Summary: This project was designed to address the question, "*Do visualizations really help students learn*?" The investigators compared and evaluated available molecular visualization software programs that are used widely by instructors in biochemistry, biology, chemistry, and related disciplines. A cognitive psychologist critiqued assessment instruments and provided guidance in the analysis of assessment data. The project investigators participated with others in developing a research plan to investigate the teaching of biochemical concepts and scientific thinking skills by interactive investigation of the properties of hemoglobin.

4. The influences of external representations on introductory chemistry student's learning of particulate structures and processes

Principal Investigator: Mark Walter, Oakton Community College
Co-Principal Investigators:
Dorothy Gabel, Indiana University
David H. Uttal, Northwestern University
Zafra Lerman, Columbia College, Chicago
John K. Gilbert, The University of Reading, UK
Contact: Mark Walter, mwalter@oakton.edu

Summary: This minigrant initiated a collaboration that focused on using students' explanations of self-constructed external models to monitor conceptual change and the influence of the external representations on this process. The work involved studying the effect of allowing students to create atomic and molecular models from pliable, nontoxic Play-Doh. The project conducting experiments to compare the Play-Doh visualization tool with a visualization created using pen and paper and explored the contributions of cognitive psychology to understanding the Play-Doh visualization. The visualization experiments were conducted at Oakton Community College and Indiana University, Bloomington. The results, though preliminary, showed enhanced learning when the Play-Doh visualization method was used.

5. Peer-led chemistry workshops as testbeds for new visualizations in organic chemistry

Principal Investigator: Carl C. Wamser, Portland State University
Co-Principal Investigator: Neil Stillings, Hampshire College
Contact: Carl Wamser, wamserc@pdx.edu

Summary: This project created new visualization exercises and assessments on stereochemistry for organic chemistry courses. The new materials were tested with students in peer-led team learning (PLTL) workshops in the organic chemistry class at Portland State University. The assessment of student learning emphasized mental rotation skills judged by student scores on standardized tests for mental rotation as well as on course-based stereochemistry problems. The project developed instruments to investigate correlations between student success in understanding and applying stereochemistry in an organic chemistry context with a more general ability to perform mental rotation of three-dimensional objects. New molecule-based mental rotation tests were developed and have been tested in the PLTL workshops.

6. Visualization to promote conceptual change

Principal Investigator: Vickie M. Williamson, Texas A & M University
Co-Principal Investigators:
Guy Ashkenazi, Hebrew University, Jerusalem, Israel
Roy Tasker, University of Western Sydney, Australia
Contact: Vickie Williamson, williamson@tamu.edu

Summary: The participants in this project developed a web-based instrument, collected research data with that instrument, and investigated whether video demonstrations or molecular animations helped students to understand chemistry concepts and if the order of presentation of the macroscopic video or animation affected learning. Students showed improvement after each visualization. A significant improvement in responses was seen between the first and second visualization. These results were interpreted to mean that it is important to combine both types of visualizations, but that the specific order may not be important.