Alex Johnstone suggested that chemists view their field within a triangular matrix of ideas (Figure 1).\textsuperscript{1,2} We observe physical and chemical changes and make quantitative measurements. These macroscopic observations are codified in symbols, in the form of chemical or mathematical equations. In this regard we are much like musicians who hear music and represent it on paper in the form of notes with an indication of time and key. But chemists go beyond this by trying to visualize what we see and symbolize by using models of chemical behavior on the particulate or atomic and molecular level. These visualizations can take the form of physical or computer-drawn molecular models or computer-generated animations.\textsuperscript{3} It is the computer that has opened up the atomic and molecular level to visualization by chemists and their students.

![Figure 1. Chemists think about chemistry within a triangular matrix of ideas. Computers can enhance chemistry instruction by illustrating the particulate view.\textsuperscript{3} (Used with permission from Saunders College Publishing.)](image-url)

Computers can clearly lead to enhancement of chemical education as they can be used by individuals or classrooms of students to view photos, graphics, movies, and animations of chemical phenomena, material now readily available from publishers,\textsuperscript{4} on the internet,\textsuperscript{5} or from sources such as the \textit{Journal of Education Software}. Molecular modeling software is also becoming less and less expensive, and faculty are finding innovative ways of using it in courses beginning with general chemistry.\textsuperscript{6} Discovery-based learning is now much more feasible, with several very successful experiments currently underway.\textsuperscript{7}
Our interest in using computers in chemical education began about 10 years ago. It was clear even then that, appropriately applied, computers had the potential of opening up new insights for students and helping them become more involved in the learning process. Our activity in this area has been in four areas:

- software development;
- use of images, videos, and animations in traditional lectures;
- use of interactive software in tutorials;
- and use of computer-based molecular modeling in upper level courses.

Software Development

In 1991-1992 I spent a sabbatical leave at the Institute for Chemical Education (University of Wisconsin-Madison) working with John Moore, Paul Schatz, and Jon Holmes in developing a hypertext “textbook” of the chemistry of the elements. The history of discovery of each element is described, along with a description of its chemical and physical properties; all of these are illustrated with photos and videos of reactions, photos of the discoverers of the elements, and molecular structures. Now called the Chemistry Navigator (Macintosh) or The Illustrated Periodic Table (Windows), the program is used by my students as a way to uncover information on the chemical elements for a weekly “chemical puzzler” in our general chemistry course. It is also used to supplement a laboratory experiment on the chemistry of the elements.

One lesson learned from the development of the Chemistry Navigator is that successful, large-scale software development cannot be done by an individual; a team approach is required. Thus, our other large project—The Saunders Interactive General Chemistry CD-ROM—involves over twenty writers, photographers, programmers, designers, and researchers, as well as William Vining and myself, the persons listed as the authors of the program. This program is now used worldwide and is the basis of my lectures and tutorials.

Computer-Enhanced Lectures

For many years I taught general chemistry using pre-made overhead transparencies. I uncovered the material point-by-point on an overhead projector and illustrated as many concepts as possi-
ble with live chemical demonstrations. Thus, it was only a small step to move to doing all of my lectures by computer using Microsoft PowerPoint™, lectures that now incorporate the videos and animations from the Saunders Interactive General Chemistry CD-ROM. (Examples are available in the form of pdf files in the U.S. at http://www.oneonta.edu/~kotzjc or in New Zealand at http://www.che.auckland.ac.nz/Stage1/Courses/410150/JKotz/JKHome.htm.)

It is important to notice that the PowerPoint slides are not simply a list of statements (Figure 2). Rather they include videos of chemical and physical changes and animations of these processes on the atomic and molecular level. (These run from the Saunders Interactive General Chemistry CD-ROM when the slide is opened or, if the latest version of PowerPoint is used, they can be triggered by a mouse click.) Also used in the slides are molecular models (available on our CD-ROM or constructed using the molecular modeling software from Oxford Molecular), images found on the World Wide Web, or original drawings. The intention is to enrich the lectures as much as possible with visual illustrations of chemical phenomena and representative molecular structures. It is intended to remind the students continually of the triangular matrix of ideas by showing chemical and physical changes, by showing how those are symbolized by chemists, and by modeling these phenomena at the atomic and molecular level.

Although the usefulness of presentation programs such as PowerPoint is now evident to many in the chemical community, some may believe it is a passive environment. Rather, we believe it is an enriched environment. I have found that, before showing a video or animation or a slide of information, it is best to develop the ideas on the blackboard. The PowerPoint slides are used to summarize the idea, show it more accurately, or expand on it. In addition, the demonstrations shown in Quicktime™ movies (or on laserdisc or videotape) are also done “live” as often as pos-
sible so the students have a sense of time and scale.

It is important to promote, as much as possible, an active environment during lectures. For this reason students are given sheets of short questions or problems in almost every lecture. We pause during the lecture several times for them to work with their neighbors to answer these questions. I walk around the room during these periods to help them and to assess their progress. Students hand these in for extra credit.

A question often asked about the lectures is if students still take notes when the lectures are laden with graphics. We give students sufficient time during the lecture to make notes, and a cursory examination of their notes indicates that they do indeed sketch important graphics. In addition, we are developing exercises that help students learn to make meaningful sketches of molecular structures.

One way to assist students in note-taking has been developed at the University of Auckland. There students in the general chemistry courses are given “lecture shells,” a set of incomplete course notes with spaces for them to add information from the lecture. In my lectures at Auckland I gave students shells that contained the key PowerPoint slides, often with important points missing, however. Next to each slide was a space to add additional information. In addition, questions were often added that would prompt class discussion or that could be the basis of an examination question. For example, the lecture shell question associated with Figure 2 asked students to explain how heat energy and molecular motion are related.

If we are to present chemistry in an enriched environment, students need to be examined in the same environment. Therefore, the examinations in my course now include questions that can only be answered by watching an animation or video demonstration. For example, after watching a short video of an experiment involving the diffusion of bromine vapor in air and in a vacuum, students are asked to describe their observations and explain why the diffusion rates are so different in the two experiments.

Finally, it is very important that rooms for computer-enhanced lectures be properly designed.
The classroom in which my lectures have been held has two computers (one G3 Macintosh and one Windows computer), a laserdisc player attached to each computer, a videotape player, a very good stereo sound system, and two RGB projectors, one for the computers and a second one for the disc and tape players. In addition, there is generous blackboard space and an overhead projector. Of particular importance is the room lighting. It must be designed so that the projector screens are not lighted by room light. At the same time the seating area has to be well lighted so that students can take notes. These conditions are difficult to achieve and may be the most costly item in renovating lecture space.

**Interactive Software in Tutorials**

Our General Chemistry course includes three lectures each week and a one-hour recitation or tutorial session for groups of up to 24 students. (There is also a three-hour laboratory session.) Previously students came to these sessions to ask questions about homework and to review the weekly lectures. With time, however, these seemed less effective for a number of reasons. Presently we use the *Saunders Interactive General Chemistry CD-ROM* as the basis for exercises that accomplish many of the same objectives as before. The students come to our Chemistry Computer Laboratory where they work *in pairs* on questions and exercises based on the material on the CD-ROM. The questions are those in the *Workbook* that accompanies the CD-ROM or modified versions of these questions. I circulate around the room, helping the slower students and encouraging the better ones. Every 10 minutes or so we try, as a class, to come to a consensus on an answer or conclusion to the exercises. In a 50-minute class, students can work through 3 to 5 exercises.

I believe this approach has been successful. Not only is attendance at the weekly sessions greater than before, but comments from students overwhelmingly indicate their approval. One of the most interesting comments came from a student who noted that her retention of course material was better in this environment than in a more traditional lecture course. This is significant, but it could of course arise from a number of causes and may only be her perception. Nonetheless, it is a testable statement and one that is important to test if technology-enhanced courses are to be developed further.
Computer-Based Molecular Modeling

About ten years ago CAChe Scientific, now Oxford Molecular, marketed a powerful molecular modeling tool. Although extremely expensive at the time, it was ideally suited to teaching inorganic chemistry in particular because it was the only such system that could be used to construct unit cells of solids. After receiving the system as a grant from CAChe Scientific, we incorporated the system first into an inorganic chemistry laboratory course and later into advanced inorganic chemistry and a lower level descriptive inorganic chemistry course. Some uses are now also being made in general chemistry.

In the laboratory course the students spend 6 to 8 hours on an experiment. They use the software to model a molecule of the substance to be prepared and to predict some of its properties (e.g., its infrared spectrum). After preparing the substance in the laboratory they use the software to explore further the properties of the molecule and/or to confirm some of their experimental findings.

One experiment involved the synthesis of \((\text{Ph}_3\text{As})_2\text{Pd}(\text{SCN})_2\). The problem was to decide if the SCN\(^-\) ligand was N- or S-bonded. Experimentally, one can tell the mode of bonding by examining the infrared spectrum of the SCN\(^-\) ligand: the CN frequency decreases if it is N-bonded and increases if it is S-bonded. [This result can be predicted if one calculates the infrared spectrum of a simple complex of SCN\(^-\) (we used AlCl\(_3\)(SCN) as a prototype system).] To get some insight into the expected bonding mode the students calculated the molecular orbitals of the SCN\(^-\) ion to discover whether the HOMO was located on the N or S atom. They also calculated a surface that represented the susceptibility of the SCN\(^-\) ligand to electrophilic attack. All signs pointed to S-bonding by the ligand, a result confirmed by infrared spectroscopy of the prepared complex (and backed up by the calculated spectrum).

In the lecture courses on inorganic chemistry students use molecular modeling to visualize structures, measure bond angles and bond lengths of typical molecules, and construct unit cells of standard solids, among other projects. All examinations in these courses are “take-home examinations” and all involve questions that can only be answered using molecular modeling.

Summary

“Our technologies for representing reality have always constrained the questions we could pose and the things we could teach.” This statement appeared in *Campus Tech* magazine in 1993 and
I believe illustrates the potential impact of computers on chemical education. Blackboards and textbook did indeed constrain the questions we could ask. Now, however, we can hope to give students deeper insights into chemistry, certainly at the atomic and molecular level.

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REFERENCES

5. Following is a small selection of useful URLs for chemical education.
   (a) ChemDex, which includes Web Elements, the best site on the World Wide Web about chemistry: http://www.shef.ac.uk/~chem/chemdex/ or http://www.webelements.com
   (b) The NIST Webbook: http://webbook.nist.gov. This is the site run by the U.S. National Institute for Standards and Technology. It is the authoritative database of information on chemical compounds.
   (c) The American Chemical Society's site for access to information: http://www.chemcenter.org/
   (d) Materials Safety Data Sheets (MSDS): http://research.nwfsa.noaa.gov/msds.html
   (e) *The Journal of Chemical Education*: http://jchemed.chem.wisc.edu/
The Yahoo! Chemistry Directory. An excellent starting place for searching the Web for chemistry-related materials and information: http://www.yahoo.com/science/chemistry

The Comic Book Periodic Table: http://www.uky.edu/~holler/periodic/periodic.html

RasMol and Chime: http://www.umass.edu/microbio/rasmol. This site contains links to support files for the two molecular viewing applications, Rasmol and Chime. There are tutorials on using the programs and links to other modeling sites.

6. Several recent articles in this area are:
   (c) H. Ungar, Syllabus, May, 1999, pages 53-56


9. Microsoft PowerPoint™ is a good choice for this activity as it is widely used, can be used after relatively little training, can be used for adequate presentations at the simplest level, or it can be used in a very sophisticated manner. Finally, the presentations can be converted for running on the World Wide Web. Other presentation packages are also available.


11. In one survey, 55% of the students strongly agreed that the format of the computer-enhanced course was conducive to learning chemistry; 34% agreed and 11% were neutral. None disagreed. A few examples of other relevant comments were:
   (a) “Using the CD and computers for more student-centered learning versus lectures would improve learning in chemistry.”
   (b) “The most effective use of multimedia is through integrating the movies and [animations]
with the lecture material.”

(c) Multimedia “can show things that can’t be explained as well in a textbook.”

(d) “The 3D graphics on the CD helped in spatially picturing chemical structures in my mind.”

(e) The “multimedia devices were incredibly helpful .... They made the lecture and text materials easier to understand by making some of the abstract theories more concrete. Especially helpful [to understand] orbitals... .”


13. An experiment has been developed that allows students to learn for themselves the principles of VSEPR theory. A copy of the experiment can be found as a pdf file at http://www.oneonta.edu/~kotzjc/GenChem.html