Visualizations in Teaching Chemistry

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Abstract: Acquisition and mastery of chemistry concepts depend on an interpretative framework that is microscopic and requires a three-dimensional dynamic representation. The Visualizations in Chemistry project created a computational environment where students can do simulations of atomic and molecular bonding in order to develop a more intuitive understanding of quantum chemistry. Students used a high performance computing environment to perform calculations and interactively visualize the resulting images. In this paper, we report on one detailed implementation where 7 conceptual areas were evaluated. The results showed improvements in students' visualizations of atoms and molecules, but it was not clear if the students' initial models were replaced. Suggestions for future implementation include more attention to learning in the visual mode, more chemistry background preparation, and use of an improved interface.

The Motivation

This project, Visualizations in Teaching Chemistry (ChemViz), grew out of the quest to discover ways to render certain basic concepts of chemistry more vivid and visible to young learners. Due to the microscopic nature of chemistry, many of its basic constructs and processes are "invisible" to students. The project's original principal investigator, Dr. Nora Sabelli, a professor of chemistry, pointed out the contrast between chemistry and physics and biology education (Sabelli, 1995):

> In physics and biology, mechanistic simulations have been used and studied extensively, whereas in chemistry we cannot draw on students' previous intuition to aid in their understanding. We all learn over a long time the intuitive skills needed to count, measure, gauge speed and force, understand motion, birth, death and growth, among other concepts. These concepts (and associated misconceptions) are macroscopic in nature and therefore observable; this is not true of many of the basic concepts of modern chemistry as it is taught now, even at the introductory level. When we see chemical reactions (cooking, moving cars, sun-burning, healing) we do not see what we are taught in chemistry and therefore, often enough we do not see 'chemistry' at all.

Historically, chemistry educators have tried to render chemical structures and processes more visible through the use of vivid, albeit excessively simple, visual metaphors such as the solar system serving as a model of the structure of an atom. While marginally useful in early stages of learning, such metaphors eventually interfere with a rich understanding of basic chemical concepts. More recent pedagogical work has suggested that computer-generated three-dimensional animations of certain basic processes, molecular bonding for example, are capable of providing students with this type of richer visualization (e.g., Sabelli, 1991). It has also been suggested that such visualizations help students obtain a better grasp of the abstract aspects of chemistry, such as calculating algorithmically-based solutions to problems.

Building on these more recent findings, the investigators of the project proposed a pedagogical approach that starts with a *computational experiment* on an abstract concept, and then proceeds to present the model (the visualization) to interpret the experiment. The computational experiment approach allows, in contrast to theory and experimentation, students to *explore* how the "laws" of chemistry behave. In a computational experiment students can do simulations which visually and dynamically replicate the behavior of a complex chemical process. An example, prevalent in this project, is the numerical solution to the Schrödinger equation. In a computational experiment, students learn by doing because they can manipulate their learning environment, testing different computations against models in an iterative fashion.

In order to explore this pedagogy, the investigators proposed to develop tools that would allow both teachers and students to do the simulations and visualizations easily and routinely so that the students develop an intuitive understanding of the chemistry "laws" behind the models.

Besides computation and visualization, a third pivotal piece in this approach is access to a high-performance computing environment (e.g., a Cray supercomputer) to conduct the simulations and create the images in time-frames (a few seconds of computing time) that make the manipulations feasible and at least theoretically useful from a pedagogical perspective.

The Substance of ChemViz: Teaching & Learning Abstract Chemical Concepts

The ChemViz (an abbreviation of the term "Visualization in Chemistry") project was and continues to be a curriculum materials development project wherein the computational approach to chemistry is used. The unique aspect of this approach is the use of a high performance computing environment to obtain images and animations of the atoms and molecules being studied.

The project members believed the computational approach would have a revolutionary impact on the high school chemistry curriculum. This approach would allow high school chemistry students to use the supercomputer as a laboratory for designing experiments which would answer their questions concerning such abstract concepts as electrons, atoms, molecules, and chemical bonding. By generating images of the electron densities for various combinations of atoms, students would be able to understand in concrete terms the differences between equal and unequal sharing of electrons, bonding and anti-bonding orbitals, strong and weak bonds, and the energy differences of atoms at appropriate and inappropriate bond distances and angles. Virtually any concept involving chemical bonding could be explored using the computational tools.

To give the reader some idea of the chemistry concepts involved in ChemViz, sections describing the popular models for teaching molecular bonding are presented here and are followed by a section more specifically related to ChemViz and its approach to bonding.

Models of the atom

Currently, chemical bonding is taught in a variety of ways at the high school level. In most high school classrooms, the Bohr model of the atom is used to introduce students to the concept of energy levels. This model is the picture that most non-scientists have of the atom: a hard ball as the nucleus with tiny electrons whizzing around it in defined orbits. This is an incorrect model, but it is the first thing explained to students because it is easy to understand and introduces the concept of quantization of energy. The Bohr model, however, cannot be used to explain bonding.

At some later point, the Bohr model is replaced by the electron cloud, or Schrödinger wave-mechanical, model in which electrons are no longer considered as being located at a given distance from the nucleus, but are instead described as having a finite probability of occupying certain regions around the nucleus. High school students are more successful at visualizing the Bohr model of the atom because it is more concrete. The Schrödinger wave-mechanical model is more difficult for high school students to visualize. It often requires some understanding of probability, 3D geometry, wave-particle duality, and quantum mechanics.

Molecular Bonding Models

The models of chemical bonding are all based on the Schrödinger wave-mechanical model of the atom. Two common terms used in these models are valence electrons (or the electrons which occupy the outermost principle energy level) and core electrons (or the electrons in an atom which are not in the outermost principle energy level).

The simplest of the bonding models is localized electron/ionic bonding model. It is based on two concepts: the atoms in a molecule are at the lowest energy when the atom's outermost occupied principal energy level has achieved a noble gas configuration. Thus, in forming molecules atoms interact with each other to share, gain or lose enough electrons to achieve this. Second, the atom tends to gain, lose, or share electrons according to a property of elements called electronegativity, which is a relative measure of the atom's ability to attract electrons shared in a bond to itself. This model is very good for predicting shapes of molecules, and for getting a general idea of the bonding. However, it cannot predict bond distances or energies, and cannot explain some phenomena such as paramagnetism.

Molecular orbital theory addresses a problem with the localized electron model: it allows the electrons to be delocalized throughout the molecule (thus avoiding the problems of resonance). In molecular orbital theory, two atomic orbitals overlap and split into two separate orbitals, one bonding and one anti-bonding. Electrons which are placed in the bonding orbital contribute to holding the molecule together, while those placed in the anti-bonding orbital to destabilizing the molecule. This theory avoids the problems of resonance and can be used to explain many phenomena, like paramagnetism. However, it is unable to explain shapes, and bond lengths. It is also difficult to apply to a molecule with three or more atoms.

ChemViz uses the self-consistent field theory to calculate the orbitals and energies of molecules. Given the positions of atoms and the mathematical representations of the atoms (called basis sets), it then calculates the possible interactions of the electrons. Using this set of calculations, it recalculates, continuing until it gets two sets of calculations which agree with each other ("self-consistent"). From the calculations, then, mathematical descriptions of the molecule's orbitals and energy can be produced. This model is the most sophisticated of all those discussed here. Though it gives very accurate results, it has two major drawbacks. First, to use this model, one needs a supercomputer to do the calculations. Second, the computer can only do calculations for the positions you give it; there is no direct way of getting the best configuration for a molecule from only the types of atoms in the molecule.

Description of the Interface, Chemistry Software and Related Programs

For a student to obtain images to model the bonding process, a set of programs are used. First, the student uses the interface program, Boogie, to set the desired parameters and create the input file which will be sent to the Cray supercomputer. Boogie presents the user with a periodic table, from which the atoms of interest are selected. The user then defines such parameters as the coordinate of the atoms, which will define the distance between the atoms in angstroms and the bond angles, and the charge on the group of atoms. For example, if a student wanted to model the water molecule, he would determine the positions for the oxygen and hydrogen atoms, then use Boogie to create the input file and send it to the Cray.

The Cray supercomputer uses DISCO, a research-level chemistry program, to do the calculations based on the input file from Boogie. The resulting output files are automatically returned to the student's personal computer. In order to view the output files as images, the student uses the imaging program NCSA Collage, which creates three-dimensional graphical images of the probability densities. The student can also analyze the output file containing the calculated energies of the molecule or molecules modeled using the program Graphical Analysis, by plotting a graph of energy vs. atom-atom distance.

DISCO is a set of FORTRAN programs that determines the molecular orbitals, electron density, dipole and quadrupole electric moments, and equilibrium structures of molecules (or atoms), ions or radicals. These properties are determined by the DIrect SCf Optimization (thus the name DISCO) method of solving the Hartree-Fock (quantum mechanical) equations. DISCO also contains a program that estimates the electron correlation energy from second order perturbation theory.

Because the user is able to specify exactly how he wants the atoms placed and can create series of images to examine how the orientation of the atoms affects the bonding of the molecule, he cannot only view the electron densities of a molecule, but can also observe the changes in the electron densities of a group of atoms as they are moved, obtain energy values for each configuration in order to compare the relative stabilities, determine the equilibrium structure of the molecules by finding the conformation with the lowest energy, and determine the dipole and quadrupole electric moment.

Major Study Questions

Two major questions guided the evaluation, with a third embedded question.

1. How does *learning* change as a function of this new approach to teaching atomic and molecular bonding?

2. How does *teaching* change as result of using ChemViz materials in the classroom?

Embedded within each of these two overarching questions is a third pervasive question:

3. Should *high performance computing* be used in the high school classroom for improving the teaching of chemistry?

Such an advanced computational approach requires substantial support in the technical and communication aspects, especially for the fieldtesters. What is the value added to students' learning and what are the benefits and costs to teachers in this effort to integrate advanced technology and chemistry education?

A ChemViz Implementation

This is just <u>one</u> of the case studies of the ChemViz project. This case study is selected as an exemplar and because it is the more detailed study. Each case study varied and the common findings among them will be presented briefly at the end. What we want to do here is to give an idea of a specific implementation.

David Bergandine teaches chemistry at the University High School in Urbana. In May, 1993, an experimental study was designed to observe any changes in learning that would be obtained by emphasizing scientific visualization without requiring students to use the computer. Available for this study were three classrooms of first year (sophomore) chemistry students, for a total of 47 students. Over the course of three weeks a series of lessons and activities were performed using the images and animations to teach atomic and molecular bonding. For assessment purposes, the students were given a pre-test before beginning the unit and a post-test at its conclusion. For comparison purposes, the two tests shared seven common conceptual areas (denoted by a *). The concepts tested were: Periodic table use, Understanding of the atom, *Atom visualization (through drawing), *Lewis structure drawing (for atoms), *Understanding of the thermodynamics of bonding, *Lewis structure drawing (for molecules), *Molecule visualization (through drawing), *Understanding of "He_2", Understanding of a larger diatomic molecule (N_2, O_2, or F_2), and *Understanding of a non-diatomic molecule (HF).

Results

The pre- and post-test analysis of the 7 common conceptual areas are summarized in Table 1 below. Each of the conceptual areas is then discussed in detail.

Conceptual Area	Pre-test	Post-test
Atom Visualization (see note 1)	5%	5%
Lewis structure drawing (for atoms) (see note 2)	87%	49%
Thermodynamics of bonding	33%	44%
Lewis Structure Drawing (for molecules)	53%	68%
Molecule Visualization (see note 1)	0%	18%
Understanding of "He_2" (see note 3)	0% (38%)	51%
Understanding of a non-diatomic molecule (HF)	4%	24%

1. Defined as drawing an electron "cloud"
2. The numbers may be misleading, as there was only hydrogen on the pre-test, and there were also helium and fluorine on the post-test.
3. None of the students could produce the non-visualization answer on the pre-test, as they were not shown the pictures. The pre-test number in parentheses represents the percentage of students who gave the traditional answer.

Table 1: Percentages of Students who Demonstrated Proficiency in the Areas Tested on the Pre- and Post-tests

Atom visualization

The results of the analysis of this section were overwhelmingly negative. 86% of the students drew atoms as nuclei with electrons in circular orbits around them. This is to be expected, especially if the students have discussed the Bohr model of the atom. The discouraging fact is that seven of every eight of those students drew atoms in exactly the same way after using ChemViz. Only one of the thirty-eight students who began the program with a drawing a circular electron orbit abandoned that view completely, and four of the students drew both a picture of a circular orbit and a picture of an electron cloud. Three students began the program drawing electron clouds (one of them also included a drawing of a circular orbit), but only one of them retained that picture. Another drew only a circular orbit on the final exam, and the third drew very unusual dumbbell-shaped orbits.

Lewis structure drawing (for atoms)

This quality was more difficult to analyze, due to the fact that the only element for which the students were to draw a Lewis structure on the first exam was hydrogen. Most of the students (87%) did do well at this, but it is a very simple task. More enlightening is how the students who drew hydrogen correctly responded to the symbols question on the post-test. Of these thirty-nine students, slightly more than half of those students did well in drawing all three of the requested elements on the post-test (hydrogen, helium, and fluorine). Additionally, one in six did well on hydrogen and helium, but made mistakes on fluorine (normally putting all nine of its electrons in the valence shell). The remaining students (slightly less than one in every three), drew either poor Lewis structures or none at all, even though the question was worded in a similar fashion.

Understanding of the thermodynamics of bonding

This was a very difficult area of knowledge to assess accurately for two reasons. First, the range of minor misconceptions that the students had was wide, and very few misconceptions were held by more than two or three students. Clouding the issue further, it was often difficult to tell if a student who answered the questions poorly did so because they were confused about the topic, or because even though they understood what was supposed to be going on, they had trouble putting their ideas into words. For those reasons, then, responses were classed based on evidence of significant improvement across the exams in the student's concept of the thermodynamics of bonding. Twenty-nine of the forty-three students (67%) had significant flaws in their conceptions when they took the pre-test. Nine of the twenty-nine (31%) gave answers on the post-test that showed a good understanding of the thermodynamics of bonding. The rest of the students showed varied stages of increased comprehension, from minor to none, and, unfortunately, there were even four students who seemed to regress.

Lewis structure drawing (for molecules)

Lewis structure drawing was an area in which the students appeared to improve significantly. The post-test showed a 28% increase overall in students who were able to draw good structures, from just over half of the total students on the pre-test to better than two-thirds on the post-test. Additionally, students appeared to rebound from common mistakes with a fair degree of success. The most common mistake (one in every five students) on the pre-test was miscounting the total number of electrons in the molecule. This did not seem to be a real problem, as most of the students were able to correct it on the post-test. The second most common mistake (roughly one in six students) was a failure to surround each atom in the molecule exactly eight electrons, and five of the eight students were able to correct it on the post-test. There is one negative aspect, however. Less than three quarters of the students who were able to draw good structures on the pre-test did the same on the post-test. It is not clear whether this has anything to do with ChemViz. It is curious nonetheless that 28% of students who did well on the first test did not on the second, and 64% of those who did not do well on the first test did on the second.

Molecule visualization

The results of this section were very comparable to the results of the atom visualization section, although students were more successful here, in that just over half of the students maintained their original image (as opposed to seven in eight in atom visualization). The most popular misconception was that the hydrogen atom looked like two protons with electrons in planetary orbits which happen to touch each other. Nineteen of forty-nine students drew this type of picture on both the pre and post-tests; however, there was a total of twenty-eight such drawings on the pre-test, and twenty-four on the post-test. This is an improvement, but certainly not a marked one. The only other significant misconception was very similar, but instead of two touching orbits around separate nuclei, both of the electrons were in a planetary-type orbit around both of the nuclei. Almost one-fifth of the students answered this way on the pre-test, but only one in eight did so on the post-test. Finally, the fact that may be most noteworthy is that none of the students answered the "right" way, that is, drawing an electron cloud, on the first test, but that almost one in five did so on the second test.

Understanding of "He_2"

This was an interesting area. Only 9% of the answers on the pre-test fell outside of three major categories, and only 11% on the post-test outside of two. On the pre-test, the popular responses were that He_2 doesn't form because "the shells are full," meaning that the atomic orbitals are unable to hold more electrons, there is a law (which was never explained or named) which prevents it, and no idea. On the post-test, many students did very well at interpreting the images that they were shown. Unfortunately, many students also failed to see the image of the σ orbital for what it is, and instead said that it showed that the molecule did not bond. An interesting observation about the tests was made: When the students were discussing the roles that orbitals play in the formation of a molecule, they tended to use the word bonding instead of combining (or a similar word), indicating that they did not recognize that the original *s* orbitals lose their individual identities when a molecule is formed.

Understanding of a non-diatomic molecule (HF)

The results of this section seem to show primarily that, given a choice, students far prefer to draw Lewis structures instead of other types of pictures. However, since that is a rather subjective judgment, data about the students' conceptions is based solely on what they have drawn. From that, it seems that there are some good things going on here. One quarter of the students ended the unit correctly representing HF as a polar covalent molecule. This is a 550% increase from the beginning of the unit. There was also no regression from the "correct" answer, which is encouraging. The only significant misconception (three out of four on the pre-test, over half on the post-test) was that HF is a nonpolar covalent molecule, and this is not too far from the truth. Some students (one in twenty on the pre-test, one in ten on the post-test) went to the other extreme of the bonding continuum and represented it as ionic.

Conclusions

Based solely on this data, there appeared to have been improvement in the students' knowledge of chemistry, but the most significant improvement came in areas which were not the focus of ChemViz. Of those areas which appear to be "targeted", visualization of atoms and molecules, there was very little improvement. This is certainly not to say that ChemViz is not useful. The students did improve their understandings of the thermodynamics of bonding, Lewis structure drawing, and the concept of polar covalency.

ChemViz was likely very helpful in these areas. It includes a feature that allows the energy of a system to be determined, and the energies of a time series (such as two atoms moving closer together) can be animated. This feature was surely useful in demonstrating the thermodynamic phenomena that occur as atoms approach. Through images, ChemViz can also demonstrate the three types of bonding in a molecule (nonpolar covalent, polar covalent, and ionic). The students in this class seemed to pick up well on distinctions between the three. In summary, ChemViz would be a useful classroom supplement for covering these topics; most students showed improvements in their understanding of these concepts. ChemViz was also very helpful to a few students in changing the way in which they think about atoms and molecules, but the number of students affected in this way was minimal.

Overall Results from the ChemViz Project

The full ChemViz evaluation report reflects a complex evaluation with many stages and multiple data sources. In an effort to present the overall result we will summarize the findings and insights of the various "probes" taken in a variety of implementation settings across the three years of the project. The overall analysis was done by contrasting a "perfect world" scenario of a perfect technological environment, a well-developed curriculum, a revolutionary learning environment, and a collaborative teaching environment to an "imperfect world" with all the fits and starts and glitches that come into play when real people, fallible machines, and imperfect technologies are involved.

Impact on learning

There is weak to modest evidence for the positive impact of ChemViz on learning. There were no broad overwhelming effects, such as all of the students in a class reaching an epiphany about the nature of chemical bonding by developing a clearer understanding of the process or shifting to a more complex model. Instead, there were individual cases of insight surrounded by other cases of misunderstanding or confusion. For some students, probably those with sufficient background knowledge to benefit from this approach, this environment provided just the spark they need to move to the next level of sophistication. For others, it appears to be more of the same. It is even less clear that the ChemViz environment promoted a research ethic and disposition; in fact the data would suggest that the teacher, not the program, was the key variable in promoting student inquiry.

Impact on teaching

The teachers truly went out of their way to accommodate this new technology and the learning environment accompanying it. They did give up their positions of privilege as the purveyors to adopt the more facilitative role that they must play in a discovery oriented environment. In the final analysis, they were overwhelmed by the technological barriers and hampered by the lack of instructional materials available to them. Connectivity problems were, in most cases and especially in the early phases, virtually insurmountable.

The role of high performance computing in school curricula

While this question is at the core of this project, it is impossible to answer with the data at hand. Significant time, energy, and resources were allocated to this project, and a generous description of the return was that the benefits were modest for the students and somewhat more substantial for the teachers. Nonetheless, if the same resources had been devoted elsewhere, then the participants would have been denied the learning opportunities that they gained by working in a highly experimental environment. Viewed from this perspective, the benefits of ChemViz will be not only in the specific curriculum developed as a part of the project, but in the future generations of interactive learning environments that depend heavily upon high speed communication and even higher speed data analysis techniques. In short, the full impact of ChemViz may not be known for some time.

After Effects of ChemViz

Since the time of this study we have witnessed major changes in school networking and teaching methods. Clearly the technological environment has improved and this is allowing teachers the opportunity to examine their teaching and modify their curriculum to integrate uses of technology such as ChemViz. Perhaps now we will see the major benefits originally predicted for ChemViz; perhaps the glimpses of success pointed to in this evaluation will be realized as breakthroughs in the teaching of chemistry; perhaps ChemViz will be recognized as a stepping stone to significant changes in the way we think about teaching and learning with technology.

References

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