

Hyper Molecular Modeling: Making Computational Chemistry Tangible

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Executive Summary

One of the greatest challenges in teaching chemistry at any level is communicating the nature of things that we cannot see with the naked eye. Traditional molecular model kits, while effective, do not accurately convey the dynamic three-dimensional nature of molecules. Alternatively, computer-generated three-dimensional visualizations and simulations of molecules can help students obtain a better grasp of the abstract aspects of chemistry. However, computational models lack the intuitive feel of a 3-dimensional physical model. Research has shown that students learn best when they feel a connection to the material, and science educators in particular stress “hands-on” activities. Furthermore, these software-implemented “virtual molecular models” are limited by mouse and keyboard as input devices, which act more as a barrier than a bridge to understanding these 3-dimensional structures.

MolySym’s novel multimodal molecular modeling system creates a seamless interface between a hand held physical ball-and-stick molecular model and a computer generated virtual molecular model. We call this type of molecular modeling “hyper molecular modeling” or hypermodeling. Hypermodels blend multiple modalities (tactile, force, audio, and visual), thereby improving a student’s understanding of the physical, chemical and biological changes that occur on the molecular level. In this paper we examine the critical role hypermodeling will play in the primary and secondary education system. In particular, we describe the way it makes learning fundamental physical chemistry principles easy to understand and accessible to all students, thereby changing the way students learn chemistry and improving the general level of chemistry education.

Introduction

Chemistry often deals with applying macroscopic observations to a microscopic world. Unfortunately, this leaves chemistry teachers with the difficult task of trying to somehow explain what cannot actually be seen. Since the middle of the nineteenth century, physical molecular models that could be held in the hand have been used. These hand-held models can be readily manipulated and provide an intuitive representation of molecules, and take advantage of our natural kinesthetic and tactile abilities in exploring molecular structure. However, one of the problems that arises while using physical models in the classroom is that insufficient emphasis is placed on the fact that molecules are dynamic and their motions are governed by the laws of physics. These models are not complete representations of the realities they are supposed to represent and lack some of the most fundamental qualities such as whether a given molecule is stable and the energy associated with different states. Some of the properties, such as the relative diameter of the spheres, attempt to represent properties of the atoms to a first approximation. However, this approximation leads to an inaccurate understanding of the underlying physical chemistry, which cannot be reflected in the model. Other properties, such as the bonds in typical ball-and-stick models, give a very inaccurate and confusing representation of the true nature of molecular bonds. While "real" bonds are constantly vibrating and have shapes that are determined by the diffuse nature of electrons, physical models simply show a stick of fixed length to represent all bonds. These are just a few examples of how a static, non-interactive, physical model can be limiting and in some cases even be detrimental to a student's understanding of chemistry.

Today, in addition to physical handheld models, there are software programs that attempt to simulate the energetics and other complex properties associated with molecules. These software tools can be used to assemble a virtual molecule, display its various conformational states, and rapidly calculate many properties. This combination of visualization and calculation is often called computational chemistry or molecular modeling. Computational chemistry can help teachers communicate the same basic principles of molecular systems as model kits while having the increased benefit of lessening misconceptions based on the rigidity of kits. For example, the one difference between using molecular modeling software and traditional models in regards to structures is that tetrahedral model angles are always set to a reference value of 109.5° and bond lengths are all identical, whereas a computational chemistry program can compute the real bond angles and lengths, which in some cases deviate substantially from the reference values. Again, while this may make things a little more complicated for the students to remember, it also helps lessen the number of misconceptions they will obtain due to oversimplification.

Ideally, teachers would like to exploit the strengths of both tactile and virtual models in their courses while diminishing the disadvantages. Table 1 outlines the advantages and disadvantages of tactile and virtual models.

| | Tactile Models | Virtual Models |
|---------------|--|---|
| Advantages | <ul style="list-style-type: none"> ▪ Shows connectivity ▪ Displays the real 3D in ideal state ▪ Possibility of illustrating some intramolecular interactions (internal rotation) ▪ Can test superposition of isomers ▪ Can generate possible conformer structures by internal rotation | <ul style="list-style-type: none"> ▪ Shows true arrangement plus distortions – based on real experimental measurements or computations ▪ Can change orientation and mode of display (“true” size with space fill) <ul style="list-style-type: none"> ○ Can make measurements ○ Bond length ○ Bond angle ○ Torsion angle ○ Molecular dimensions ▪ Can visualize complicated molecules (DNA, proteins) with simplifying modes of display ▪ Provides flexibility – animated vibrations (stretch, bend, internal rotation of bonds) ▪ Can generate animated reaction mechanisms ▪ Can display <ul style="list-style-type: none"> ○ Electrostatic potential maps ○ Molecular polarity ○ Attack points in reactions |
| Disadvantages | <ul style="list-style-type: none"> ▪ Is rigid (set bond lengths and angles) ▪ True molecule size and shape not accessible ▪ No feedback between the model and the user ▪ Impossible molecules can be built without the student knowing ▪ Unphysical geometries can be generated without the student being made aware of a problem | <ul style="list-style-type: none"> ▪ Mouse and keyboard are suboptimal input devices for manipulating a molecule ▪ May not grasp the 3D nature on flat computer screen ▪ No tangible interaction with the molecule |

Table 1: Advantages and Disadvantages of Tactile and Virtual Models

Today, it is possible to merge the manipulative capability of tangible models with the visualization and simulation capabilities of virtual models. This enables students to work in multiple modalities, building the capability to mentally convert between modalities, a skill that is very beneficial to scientists.

The combination of tactile and virtual models reinforce each other, strengthening a student’s understanding of the three-dimensional nature of the structures and, more importantly, ensuring that students correctly interpret what is viewed on the computer screen. This becomes increasingly important as molecules become more complex. The

student's learning is enhanced by constantly making this virtual-tactile connection as they build and manipulate molecular models.

Hands-On Computational Chemistry

This US Department of Education funded project is based on the need to make chemistry concepts more tangible and vivid to young learners. Our patented Hypermodeling technology makes computational chemistry a hands-on learning experience. Hypermodeling allows students to use physical models to interact with computer molecular visualizations and simulations. Over the past several years, advances in robotics, electronics, computer hardware, and software have made it possible to create a multimodal molecular model that is both dynamic and tactile. The tangible user interface (TUI) of the Hypermodeling system resembles a traditional ball-and-stick model but with embedded sensors and an internal communication system. This creates a direct link between the TUI and powerful computational chemistry software. As the user manipulates the TUI in his/her hands, changes to the molecule and its properties are reflected in real-time on a computer screen, providing the student with valuable feedback.

The advantage of Hypermodeling over the use of traditional molecular models lies in the direct relationship between the physical model and real-time calculated properties, as conveyed through the software. For example, the TUI alone, like a traditional model kit, will not differentiate between bonds of different lengths. However, the TUI is linked to our software simulation system, which allows the user to explore multiple graphical representations (wire, ball and stick, tube, van der Waals, and molecular surfaces) and compute dynamic properties of the system based on real-time energy and force evaluations. Direct feedback between the software and the physical model can tell a user when he/she has constructed an unrealistic molecule, when the model is in an unfavorable state, or when the model is no longer valid.

Hypermodeling provides students with a multimodal interface for molecular modeling that helps them to qualitatively approach the physical chemistry principles and the microscopic models resulting from them. Students learn more efficiently if the instructional methods and tools match their learning style and support the creation of mental images and models, therefore the ability to visualize and physically manipulate are very helpful in their learning. Students with limited background in physics and mathematics will be able to deeply understand physical chemistry principles and create the correct mental images of atomic and molecular models.

Hypermodeling also empowers instructors in teaching chemistry. The visualization tools allow students to view the chemistry at the submicroscopic level as it occurs dynamically -- providing them with a deep understanding of the underlying chemical principles that cannot be obtained by reading text or from the static representations provided by textbooks. By backing these visualization tools with computer simulation, the accuracy and validation of the visualizations can be ensured. Also, students learn more by experimenting (active learning) than by watching (passive learning). Backing the visualization with simulation allows the students to change a chemical system (e.g., the

number, type, and location of atoms in the chemical system), and to learn about the effects on the submicroscopic behavior, and on the observable macroscopic properties.

Coupling the immediacy and the tactile nature of the physical models with computationally intensive virtual models provides students with the means to investigate, interpret, explain, and discover molecular phenomena. Students need to learn to “think like a molecule”. To do this, they need to “see” what a molecule sees and “feel” what a molecule feels. Hypermodeling gives students the best and most direct view of the molecular world and overcomes historic difficulties in chemistry education.

Classroom Integration

In 1929, the Nobel Prize winning scientist P.A.M. Dirac wrote, "the underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble." Dirac was correct in this statement: the mathematical principles needed to solve problems in chemistry are known, yet solving these equations proves to be daunting for even the most brilliant members of the scientific community, let alone typical high school chemistry students. However, 80 years later, computational chemistry provides the tools to investigate even the most complicated chemistry systems, placing it at the forefront of many areas of chemical research.

By the time many of today's students enter the workforce, career opportunities will have radically changed. Many of the great scientific achievements of the last century -- such as the discovery of an expanding ozone hole and the development of antiviral drugs to help treat HIV infection -- were accomplished by chemists and chemical engineers. Today, work in the chemical sciences is crossing over into other fields, such as biology, nanotechnology, and computer science. More than 1 million new chemical compounds are being created every year, with many groundbreaking discoveries on the horizon. The chemical sciences are at the forefront of efforts to find new energy sources, improve the environment, design new materials, detect terrorist threats, create new drugs, and better understand how human cells work. We can no longer ignore the prominence of computation as one of the essential tools in the arsenal of the research chemist. Computational chemistry must be included in our list of what it means to know chemistry. Our students must be as familiar with the Schrödinger equation as they are with the ideal gas law, and must be able to perform a vibrational analysis of a compound as readily as they are able to find its experimental melting point. Likewise, especially in this day of high-stakes testing at the pre-college level, we must expect the student to demonstrate his or her proficiency in computational chemistry on end-of-course exams, AP exams, and other evaluation tools. Without that expectation, students will not be exposed to these tools and methods, and, as a result, will not be adequately prepared for careers as scientists.

Many of the topics in chemistry are difficult for students to learn, especially those related to atomic and molecular structures. For example, Lewis dot structures and their significance are conceptually very difficult. With Hypermodels, we can mathematically

calculate and visualize lone pair orbitals. Hypermodels can help students understand why some molecules violate the octet rule. Without Hypermodels, students have to take it on faith that not all molecules follow the rules. In looking at bonding, students can perform molecular and natural bond orbital calculations and visualize sigma (σ) and pi (π) bonds. In reaction kinetics and thermochemistry, we can use Hypermodels to determine the activation energies (E_a) of a reaction, and determine the rate constant for a particular reaction. We can use Hypermodels with our organic chemistry students to help them develop a more intuitive feel for organic structures and functional groups, and perform computational experiments to determine the pKa values for acids and bases. Hypermodeling can be integrated into chemical education at all levels.

Conclusion

Research in the chemical sciences must remain ambitious if the United States is to maintain its scientific and technological leadership during this century. The field must attract the very best minds, which means recruiting more women and minorities and revising undergraduate and high school curriculums to make chemistry more appealing to students with a variety of interests. MolySym recognizes the importance of a well-educated and capable workforce and the importance of investing in technology and programs that perpetuate this. To this end, we believe bringing computational chemistry into the high school classroom will lead to students achieving higher levels of molecular literacy.

The MolySym's flagship product, the Hyper Molecular Modeling System, improves student's understanding of physical, chemical, and biological changes that occur on the molecular level by coupling a tactile representation of a molecule to the underlying digital information contained in a computer generated virtual molecule. By enabling students to get their hands on the subject matter and to work in multiple modalities, MolySym's technology provides for a deeper understanding of the dynamic nature of molecular systems. By integrating Hypermodeling into their curriculum, educators can take advantage of the technologies and techniques of computational chemistry and effectively integrate the next generation of educational tools and interactive molecular models into their teaching. The introduction of Hypermodeling into the U.S. secondary chemistry classroom will:

- 1) Increase the number of students who take advanced chemistry courses
- 2) Improve the chemistry proficiency of students
- 3) Narrow the gap between educational content and rapid advances in today's scientific understandings of molecular systems
- 4) Prepare students for future work in the chemical sciences, such as pharmaceutical, biotechnology, nanotechnology, materials, or related research areas
- 5) Increase the number of students entering fields of science related to chemistry

About MolySym Corporation

MolySym is provider of advanced technology solutions for research, training and education located in Cambridge, Massachusetts. The company emerged from the Massachusetts Institute of Technology (MIT) with a cross-section of talent from the Department of Chemistry, the Computer Science and Artificial Intelligence Laboratory (CSAIL), the Computational Systems Biology Initiative, and the Media Laboratory. We are dedicated to using emerging technologies to improve Science Technology Engineering and Mathematics (STEM) education.

For more information, visit the MolySym Corporation Web site at: www.molysym.com or contact a MolySym representative at info@molysym.com.