COLLABORATIVE RESEARCH: CONSTRUCTIVE CHEMISTRY: PROBLEM-BASED LEARNING THROUGH MOLECULAR MODELING

Summary. Chemistry educators have long exploited computer models to teach about atoms and molecules. In traditional instruction, students use existing models created by developers or instructors to learn what is intended, usually in a passive way. Almost a decade ago, NSF sponsored a workshop on molecular visualization for science education in which participants specified that "students should create their own visualizations as a means of interacting with visualization software." The lack of efficient visualization authoring tools, however, has limited the progress of this agenda. It was not until recently that molecular modeling tools became sufficiently user-friendly for wide adoption. This joint project of Bowling Green State University (BGSU), the Concord Consortium (CC), and Dakota County Technical College (DCTC) will systematically address this important item on the workshop participants' wish list. The project team will develop and examine a technology-based pedagogy that challenges students to create their own molecular simulations to test hypotheses, answer questions, or solve problems. To implement this pedagogy, the team will produce a set of innovative curriculum materials, called "Constructive Chemistry," for undergraduate chemistry courses. CC's award-winning *Molecular Workbench* (mw.concord.org), which provides graphical user interfaces for authoring visually compelling and scientifically accurate interactive simulations, will be enhanced to meet the needs of this research. "Constructive Chemistry" will be comprised of instructional units and modeling projects that cover a wide variety of basic concepts and their applications in general chemistry, physical chemistry, biochemistry, and nanotechnology. Each unit or project will pose one or more problems or design challenges that can be solved using molecular simulations and their analytic tools. For example, students will investigate why the average kinetic energy, rather than the average speed, of molecules provides a microscopic interpretation of temperature; they will discover deviations from the Ideal Gas Law as a function of the properties of the constituent gas molecules; they will design a fuel cell, a molecular sieve, or a nanofabrication procedure. The materials will be scaffolded to help students learn both science content and modeling skills, with an emphasis on conceptual understanding. Field tests will be conducted in general chemistry, physical chemistry, and biochemistry classes at BGSU, as well as nanotechnology classes at DCTC. Students' simulations and other activity data will be collected and scored to assess their learning outcomes. The software and curriculum materials will be iteratively revised based on classroom feedback. The end products will be made freely available and disseminated through the National Science Digital Library and the Nano-Link Center at DCTC. The research results will be presented at conferences and in journal publications.

Intellectual merit. Science should be taught as a verb, not only as a noun. "Doing science" is a compelling and effective way to learn. It is through the process of exploration, creation, and invention that theories are applied, ideas are tested, and knowledge is synthesized and advanced. Chemistry education involves teaching many abstract concepts that are difficult to grasp because students lack an intuitive understanding of what those concepts actually mean and how they are connected. Constructing molecular simulations allows students to learn chemistry by doing it in a process in which dots are connected, intuition is reshaped, and conceptual understanding is deepened.

Broader impacts. This project will tap into the hidden educational power of computational chemistry for supporting student design and problem solving. The results of this research have the potential to transform how computational tools are used in science education at all levels. As a by-product of this project, students at BGSU, which is a major producer of K-12 science teachers, will be exposed to the educational power of molecular modeling tools. In this way, the project will introduce those future teachers, through their coursework at BGSU, to a type of learning technology that is certain to grow in importance during their teaching careers. In addition, the partnership with the Nano-Link Center will infuse this methodology into nanotechnology programs at two-year colleges across the nation. This project will, therefore, serve as a catalyst for wider adoption of computational tools in diverse classrooms in the long run.

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> *"[The workshop] participants specified that students should create their own visualizations as a means of interacting with visualization software."* — José & Williamson, in "Molecular Visualization in Science Education: An Evaluation of the NSF-Sponsored Workshop," Journal of Chemical Education, Volume 82, p. 937, 2005

MOLECULAR MODELING FOR CHEMISTRY EDUCATION: A PERSPECTIVE

The molecular world is alien to students: Electrons, atoms, and molecules are much too small to be seen even in ordinary microscopes, and their interactions and behavior are vastly different from those of familiar objects that shape our intuitions. There is little we can offer students to manipulate directly with their hands to learn the rules of the molecular world. Needless to say, traditional static representations of molecules fall short of conveying those essentially dynamic rules.

Computer simulations can render a virtual molecular world that is visible, dynamic, and accessible to learners. The motions of atoms and molecules can be simulated using the molecular dynamics (MD) method, which calculates the positions and velocities of all atoms in the system as a function of time, based on the forces they exert on each other (Allen & Tildesley, 1987). Collective behaviors of atoms such as phase change or self-assembly spontaneously emerge from MD simulations, giving students an extraordinary predictive and explanatory tool for understanding chemistry. Although MD simulations involving many atoms often require supercomputers or hours of computation, simulations of several hundred atoms can be computed and displayed in real time on today's personal computers or even tablets. This kind of visual simulation provides an outstanding interactive learning environment that can help students develop accurate and concrete mental models essential for deep conceptualization and lasting understanding (Burkholder, Purser, & Cole, 2008; Lykos, 2004; Pallant & Tinker, 2004; Wieman, Adams, & Perkins, 2008; Xie & Lee, 2012; Xie & Tinker, 2006).

MD can be used to simulate a broad scope of chemistry topics, including gas laws, states of matter, chemical bonding, chemical reactions, intermolecular forces, heat transfer, diffusion, osmosis, nanotechnology, and so on. The fact that many seemingly disparate phenomena can be explained using only a handful of general scientific principles embodied in MD reflects the unity of science, a profundity noted by Richard Feynman in his famous lecture that opened the field of nanotechnology: "I am inspired by the biological phenomena in which chemical forces are used in repetitious fashion to produce all kinds of weird effects (one of which is the author)" (Feynman, 1992). Enlightening students with this holy grail of science is a fundamental goal of science education—it gives students powerful conceptual frameworks to integrate fragmented knowledge and thus enables them to confidently reason about new phenomena. Molecular modeling provides a means to learn how basic chemical forces are used repetitively to explain many different phenomena.

Molecular dynamics applications

Research: Molecular dynamics is an important computational tool used in contemporary research (Höltje, Sippl, Rognan, & Folkers, 2008; Jensen, 2010; Leach, 2001; Rappaport, 1997). In 2010, *Science* Magazine selected a millisecond-scale MD simulation of protein folding as one of the top ten scientific breakthroughs of the year (Shaw, et al., 2010).

Education: A number of commercial or free MD tools are available for education, including, but not limited to, *Atomic Microscope*, *Atoms in Motion for iPad*, *Atomsmith*, *Molecular Workbench*, *Odyssey*, and *Virtual Molecular Dynamics Laboratory*. Some of these tools have been widely used. For example, the free and open source *Molecular Workbench* developed by the Concord Consortium has reached nearly a million students worldwide and was awarded a SPORE prize by *Science* Magazine in 2011 (Xie, et al., 2011).

Despite its evident promise, there is still widespread skepticism about the value of using molecular modeling in the classroom. Although there have been several projects that have integrated molecular modeling into undergraduate chemistry courses and laboratories (Clauss & Nelsen, 2009; Jones, 2001; Montgomery, 2001; Paselk & Zoellner, 2002), there is no clear consensus regarding the role that molecular visualization, per se, should play in the curriculum (José & Williamson, 2005). While many teachers are excited about its illustrative power through stunning modern computer graphics, they at the same time question that molecular modeling tools would be any more useful than a mere demonstration occasionally used to aid a lecture. Their doubts are not groundless—research concerning the educational values of visualizations in secondary education has been contradictory and inconclusive (Linn, 2009; Viadero, 2007). A two-year study on the effects of molecular visualization on teachers showed that content knowledge and attitudes did not change appreciably (José & Williamson, 2008). Recent studies have further identified a problem called "deceptive clarity": While students overwhelmingly favor visualizations, they may learn only superficially from them (Linn, Chang, Chiu, Zhang, & McElhaney, 2010; Zhang, Pallant, & Xie, 2012). Molecular visualization could simply create a complacency of learning or even an illusion of understanding. How to maximally exploit the power of molecular modeling to improve student learning fundamentally and consistently remains an important question in chemistry education research.

This collaborative project of Bowling Green State University (BGSU), the Concord Consortium (CC), and Dakota County Technical College (DCTC) will develop, test, and evaluate a new pedagogy that challenges students to *create* their own MD simulations to test a hypothesis, answer a question, or solve a problem. Through this joint effort, we hope to initiate a research-based agenda to utilize this overlooked educational value of molecular modeling for problem solving and engineering design and explore how this potential can bring transformative changes to chemistry education at both two-year and four-year colleges. In the following section, we will discuss the rationale for this instructional approach based on what we know about how students learn with molecular visualization.

PROJECT RATIONALE

Almost a decade ago, NSF sponsored a workshop on molecular visualization for science education (José & Williamson, 2005), which defined the characteristics of molecular visualization that enhance learning and the type of interaction that students should have with visualizations. The workshop concluded that "simple, animated, interactive visualizations should be used by students to enhance learning of the particulate nature of matter." It also outlined the aspects of molecular visualizations that require further research, especially the need "to establish what works and evaluate what is effective."

Clarification of terminology

Throughout this proposal, the word *animation* means a planned or scripted display of a sequence of images of molecules. An animation cannot be changed once it is made. As a result, all learners will see the same animation and the same outcome when they interact with it, and learning cannot be personalized.

The words *model* and *simulation* will be used interchangeably in this proposal to mean a computational entity with which students can interact to experience its behavior. The response from the computational entity is visualized as a screen image that evolves according to the scientific principles embedded in the system in conjunction with the user's inputs. A simulation is much more powerful than an animation because it allows students to explore science through inquiry—usually in an *uncertain* and *unpredictable* way, resembling the situation in an experiment. Learning with an interactive simulation is a personal experience: each learner controls her/his own pace and manipulates the simulation in a unique manner.

Three Instructional Approaches

Basically, there are three approaches of using MD tools in teaching: observation, interaction, and construction, representing an increasing level of open-endedness and student engagement.

Observation: The first approach entails students observing an animation of a chemical process generated by a simulation tool.

Chemistry teachers increasingly use animations to help students visualize complex molecules and phenomena (José & Williamson, 2005; Russell, et al., 1997; Stueker, Brunberg, Fels, Borkent, & Van Rooij, 2003; Yezierski & Birk, 2006). Researchers have found, however, that in some cases students learn better from a series of illustrations than from an animation, because students may overlook fleeting but important details in an animation (Tversky, Morrison, & Betrancourt, 2002). In addition, the "deceptive clarity" of animations can lead students to overestimate their understanding and miss the deep scientific message the animator intends to convey (Linn, et al., 2010). The fact that using only animations in education is not consistently effective (Viadero, 2007) suggests that MD tools should not be used to generate just molecular movies or animations.

Interaction: Decades of research on multimedia learning suggest that students learn better when they interact with a computer program to make changes (Bransford & Schwartz, 2000; Feurzeig & Roberts, 1999; Frederiksen & White, 2000; Mayer, 2005; Wilensky & Resnick, 1999). The second approach for using MD tools involves students changing the variables of a pre-constructed model and observing its emergent behavior. This more effectively introduces students to the underlying concepts than simply observing animations, particularly when the interactivity is supported by a well-designed user interface that provides appropriate scaffolds. By observing the model's responses to various inputs under their control, learners more likely pay attention to causality than when passively watching an animation. This design principle is widely used in producing interactive digital media for science education (Stieff & Wilensky, 2002; Tinker & Xie, 2008; Wieman & Perkns, 2006).

A common problem with interactive learning environments, however, is the phenomenon of "gaming the system," in which students attempt to "succeed" in completing a programmed activity by exploiting properties of the system's feedback rather than by learning the material (Baker, et al., 2008). Although different categories of student interaction can be detected by analyzing the log data (McElhaney & Linn, 2011; Sao Pedro, Baker, Gobert, Montalvo, & Nakama, 2011), it is not clear how to pre-program accurate responses to discourage "gaming" behaviors without restraining legitimate search of answers.

Construction: The strongest evidence for deep student understanding comes from studies that engaged students in applying their knowledge to solve problems or design things such as robots or games (Kolodner, et al., 2003; Melchior, Cohen, Cutter, & Leavitt, 2005; Polman, 2000; Robertson & Good, 2004). Constructionism theory (Harel & Papert, 1991; Kafai, 2006; Kafai & Resnick, 1996; Papert, 1991), as proposed and practiced for more than three decades at MIT's Media Lab (Colella, Klopfer, & Resnick, 2001; Monroy-Hernández & Resnick, 2008), claims that students learn most effectively when they create their own artifacts that perform certain functions. This suggests the third approach for using MD tools: challenging students to construct their own simulations to explain a phenomenon, solve a problem, or design an engineering system. This constructive approach, which was also recommended by the NSF Workshop on Molecular Visualization (José & Williamson, 2005), represents the highest level of student engagement, inquiry, and internalization. Through an iterative process of conception, construction, test, and observation, students learn how to apply the fundamental laws, how to connect different concepts, and how to use their knowledge to design functioning systems. In a way, asking students to simulate or explain chemical phenomena using their own models is a *metacognitive* process (White & Frederiksen, 2005): It helps them realize what they do not actually understand and can spur them to revisit their models to remedy gaps in their knowledge. This learning mechanism is, in part, supported by a recent study that suggests that explaining plays a key role in cognition: When learners explicate, they learn more effectively and generalize more readily (Williams & Lombrozo, 2010). Moreover, the pride of ownership of their models tends to motivate students to pursue true understanding of the underlying scientific principles more actively (Papert, 1991), as they have to present and explain their work to others.

The Advantages of Constructing Molecular Dynamics Simulations

For novice learners, building an MD simulation offers more opportunities to learn about the behavior of molecules than drawing molecules using educational tools such as the Jmol-based *Virtual Molecular*

Model Kit (Rothenberger & Newton, 2011) or professional cheminformatics tools such as *ChemDraw* (CambridgeSoft, 2012) or *ChemDoodle* (iChemLabs, 2012). Many important concepts such as temperature, pressure, reaction, and equilibrium can only be understood as dynamic processes. To construct a virtual molecular system that shows a desired behavior involving these concepts challenges students to really understand the interactions and dynamics and learn how to put different components together to make the model work as an integrated system. For example, building a hydrogen fuel cell simulation requires that students grasp the concepts of energy, electrical current, diffusion, selective permeability, and electrochemical reactions. They must apply these understandings to construct all the components of a fuel cell model and correctly assemble them to make the model capable of demonstrating how chemical energy (bond making and breaking) is converted to electrical energy.

Unlike flipbook-like animation tools such as *ChemSense* (Schank & Kozma, 2002) and *Chemation* (Chang, Quintana, & Krajcik, 2010), with which students design animations frame by frame to reveal their understandings of chemical processes, a well-designed MD tool supports experimentation and investigation. To test an idea, students first design the initial state of a model and then run it. The calculated results are immediately visualized and images are fed back to students to help them decide whether the idea worked. Iterating through this interactive problem-solving process, students can experiment with many ideas and learn quickly from their successes and failures. In some sense, the tool serves as an interactive "tutor" whose intelligence is powered by the scientific principles built into its computational engine.

Importantly, student-created models provide instructors and researchers a "high-resolution lens" to comprehensively assess student performance. Students' design choices and models contain rich information for tracking their conceptual understandings and thought processes as they construct models.

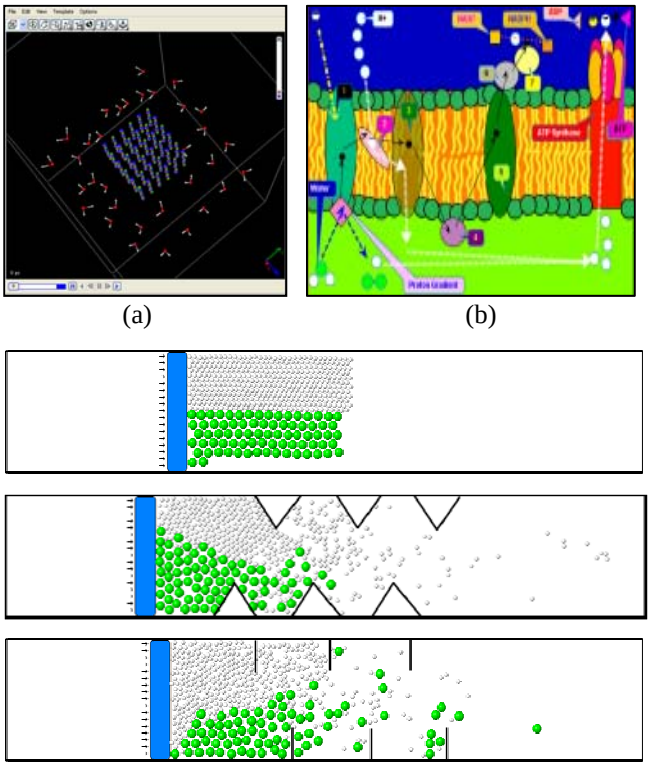


Figure 1. Samples retrieved from Molecular Workbench's database of student-created models. (a) The initial state of a 3D model created by a student at the University of Georgia (UGA) to explore dissolving of salt in water using the graphical user interface for constructing 3D MD models. (b) A photosynthesis model created by another UGA student. (c) A sequence of computational experiments designed by a student at DCTC to explore chaotic advection mixing in microchannels of different shapes. In addition, details of selected work of BGSU students can be found in the Supplementary Materials.

Broader Impacts in STEM Education

This project will contribute to the long-term effort of improving STEM education through computational models and computational thinking (National Research Council, 2010; Panoff, 2009; Wieman & Perkns, 2006). Current model-based instructions rely on models designed by developers. Ironically, the lack of strong evidence for student learning from models (Viadero, 2007) has led many to believe that the people who created the models (or other types of media) are actually the people who learned the most from them (Jonassen, 1994). Our vision of "Constructive Science" represents a bold attempt to improve model-based learning by providing students with the knowledge, tools, and opportunities to become the creators of scientific models themselves!

Although we are targeting our project at the undergraduate level, "Constructive Science"

represents a promising direction for using computational tools at pre-college levels as well. Recently, there has been encouraging progress in making software environments for easy construction of models, demonstrated by the impressive success of Algodoo (www.algodoo.com). Algodoo allows students to learn Newtonian physics through designing entertaining simulations of the real world. A similar success for chemistry will be harder (because of the lack of the macro-world counterparts for atoms and molecules and their strange behaviors), but it is not impossible. The MD method is the key to achieving the goal of delivering a similarly playful and enjoyable tool for chemistry education.

Notably, a by-product of this project will be the engagement with computational tools of students who are training to be pre-college teachers. BGSU is a major producer of K-12 science teachers. Through our project, future teachers who take the targeted courses will be introduced to a type of learning technology that is certain to grow more important over the course of their teaching careers. This project will, therefore, serve as a catalyst for wider adoption of computational tools in diverse classrooms in the long run.

PRIOR WORK

The Molecular Workbench Software

The NSF-funded[1] *Molecular Workbench* (MW) software (mw.concord.org) that will be used in this project is one of the few educational MD tools that support model construction through an easy-to-use, what-you-see-is-what-you-get (WYSIWYG) user interface (Figures 1 and 2). Furthermore, it provides a multifunctional instructional environment to scaffold and assess student learning (Tinker & Xie, 2008; Xie & Pallant, 2011). With MW, educators can pose questions for students to explore through computational experiments (Xie, et al., 2011). MW provides students access to powerful computational tools just by using clicks of the mouse. With these tools students can build models to address questions that cannot otherwise be answered without applying advanced mathematics or complex programming. This has been confirmed independently by a study that showed that even middle school students were able to design self-assembling nanostructures using MW (Shipley & Moher, 2008). The study also provided evidence for the value of the "construct-centered design methodology" in learning nanoengineering at the secondary level (The National Center for Learning and Teaching in Nanoscale Science and Engineering, 2008), which resonates with our vision of "Constructive Science."

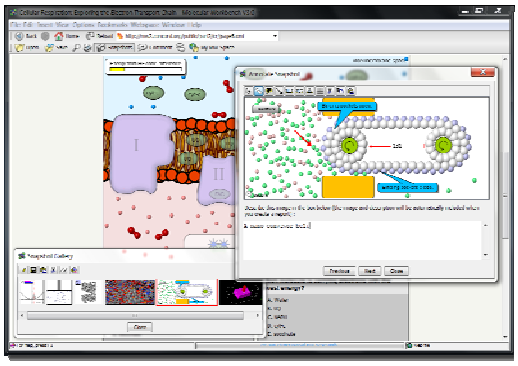


Figure 2.A screenshot of the Molecular Workbench modeling environment.

"These days, the first thing I do when preparing a lecture is to scour the Molecular Workbench for useful animations. I find animated simulations in general, and Molecular Workbench in particular, invaluable in bringing across complex concepts." — Prof. Jan Jensen, Department of Chemistry, University of Copenhagen

Another reason that MW is ideal for this research is because it provides capabilities to embed assessments in student activities and directly gather student responses and artifacts through the Internet, greatly simplifying data collection and expanding the types and amount of data that can be mined. Logged data can be used by teachers for formative evaluation of learning, which is one of the most reliable ways to improve teacher practice and student outcomes (Black, Harrison, Lee, Marshall, & Wiliam, 2003; Black & Wiliam, 1998; Horwitz, 2011).

Preliminary Results from Pilot Tests at Bowling Green State University

[1] http://www.nsf.gov/discoveries/disc_summ.jsp?cntn_id=121271&org=NSF

Excited about the potential of the constructive approach, BGSU and CC undertook an unfunded project to implement and test the pedagogy using MW in the 2008-2009 academic year. This study addressed the following questions: 1) are students able to master the authoring tools of MW in a relatively short time; 2) do the models students produce afford sufficient scientific meanings; 3) do students simultaneously learn chemistry content; and 4) are students able to apply what they learn to new contexts, for example by designing devices to solve a problem. After a year of experimentation at BGSU, we now have preliminary evidence that indicates positive results. The testimonial from a participating student provided in the box to the right summarizes well what we heard from many students.

> *"Molecular Workbench is something that I think all physics and chemistry classes should have because it gives an alternative way to grasp concepts outside of just lecturing in the classroom. It allowed me to explore in a way unimaginable before when I built a fuel cell simulation step by step myself. In essence, I could let my curiosity flow by exploring how each editing tool affected my creation. Sometimes I could not figure out how to build it myself, but the program was designed in a way that would not stop my acquisition of learning. Since it is set up like a learning community, I could view someone else's idea of how it should look. In this, I learned in two ways, by attempting my own simulation and by analyzing others."*
>
> —Britiany Sheard, BGSU student

In the pilot tests, 53 students taking physical chemistry class or independent study submitted a total of 164 models they created to simulate topics covering gas laws, ionic solutions, energetics, thermodynamics, electrochemistry, and chemical reactions. Based on the analysis of their work, we concluded that students could construct meaningful models. The examples of student work included in the Supplementary Materials indicate that this approach unleashes student creativity and helps students overcome difficulties they typically encounter in traditional approaches when trying to connect macroscopic and particulate representations of chemical phenomena (Driel, De Jong, & Verloop, 2002; Johnstone, 2000). Significantly, students were able to apply their understanding of the particulate world to situations new to them. No evidence was found that students simply copy others' models or otherwise "game" the system and, therefore, invalidate the pedagogy. Remarkably, a few students were able to come up with impressive designs that even experts had never considered before (Xie & Pallant, 2009).

The success of our pilot tests at BGSU suggests that there is great promise in this approach for chemistry education. Other institutions, including the University of Georgia and DCTC, have exploited the power of this approach independently in their classrooms using MW as well (Figure 1). A larger-scale realization of this potential, however, depends on whether the methodology developed in these trials can be captured and disseminated effectively to other faculty and institutions. One way to codify and transfer the methodology is to further develop, refine, unify, and polish our instructional materials so that they are readily transferable to others. Meanwhile, a more careful and thorough study is needed to determine what makes each strategy successful and map the relationship between modeling skills and content acquisition.

Data from larger field tests can help identify and refine the design principles for constructive curricula. Collecting and analyzing results from more students across multiple chemistry subjects at both two-year and four-year colleges will provide more comprehensive evaluation. Research is needed to identify the chemical concepts most amenable to constructionist learning and discover efficient methods for teaching students modeling concepts and skills so that they can use modeling tools effectively without sacrificing content learning for model construction.

PROJECT GOALS AND OBJECTIVES

The overarching goal of this project is to develop, test, and evaluate the constructive approach that invites students to create their own MD simulations to solve problems in undergraduate chemistry and nanotechnology courses at two-year and four-year colleges. BGSU, CC, and DCTC will collaborate to:

- **Develop curriculum materials**. This project will develop problem-based "Constructive Chemistry" curriculum materials using MW as the modeling tool. A set of learning units will be created, each covering a cluster of basic concepts in general chemistry, physical chemistry, biochemistry, and nanotechnology. In addition, a variety of modeling projects will be devised for students to undertake as homework. All the materials will be field tested and then revised based on classroom feedback. A teacher's guide will be provided for each unit.
- **Improve enabling technologies**. We will improve MW to make it significantly easier for students to construct MD models. A series of videos will be produced to help students learn how to use MW to design models. A wiki site will be set up to provide technical assistance and facilitate student discussions. Staff will answer questions and provide guidance to students through these online facilities.
- **Assess learning outcomes.** We will evaluate models created by students and the design rationale they provide to probe student cognition and the depth of learning. We will administer pre/post-tests to measure impacts of project materials. Student surveys will be conducted to add contexts to the study. A small number of randomly chosen students will be interviewed to obtain more detailed information.
- **Disseminate project materials and results.** We will disseminate our constructive curriculum through websites, digital libraries, conferences, and workshops. The research results will be submitted for publication in peer-reviewed journals and conference proceedings.

Research participants: The "Constructive Chemistry" curriculum will be field tested over a two-year period with socioeconomically diverse student at BGSU and DCTC. BGSU has a 19% minority and 30% first-generation student population (2010 data). DCTC is a two-year technical college in Minnesota, with 17% minority students and 50% female students. The project will also provide opportunities of professional development to six faculty members, four at BGSU and two at DCTC.

THE CURRICULUM DEVELOPMENT PLAN

The proposed "Constructive Chemistry" curriculum will address the conceptual difficulties or misconceptions that our team and others have identified over many years of teaching undergraduate chemistry courses (Duis, 2011; Nicoll, 2001; Rogers, 2000; Yezierski & Birk, 2006). Due to the exploratory nature of this TUES Type One project, we do *not* plan to cover every topic in the target courses. Rather, we will focus on topics where this innovation promises transformative learning. The instructional units will address basic concepts and will be used in the classroom, whereas the student modeling projects will be assigned as homework involving applications of concepts to problem solving and engineering design.

The Instructional Units

The units will be scaffolded carefully to provide sufficient guidance to students in building models using MW while leaving the exploration of science open-ended within the scopes of the topics. [Although some constructionists advocate that we should simply provide the enabling technology and let learners explore freely on their own, extensive research (Mayer, 2004; Minstrell & Kraus, 2005; Pea & Sheingold, 1987) has suggested the importance of scaffolding and guidance in open-ended explorations.] A teacher's guide will be prepared for each unit, which will include background information, instructions for model construction, sample models, links to textbooks, and additional resources. These curriculum materials are intended to complement rather than to replace lecture. Guided in-class activities will be planned to get students started with each modeling problem. The materials will help teachers demonstrate to students how to build simple models related to course topics. Students will be encouraged to share their models with each other using the MW website, articulate their design rationales, and draw conclusions regarding the phenomena they are modeling or the systems they are designing, using data from their simulations. Students' reports will allow instructors to grade their work and researchers to assess their learning.

The units are listed in the following table:

Subjects	Curriculum Units
General Chemistry/ Physical Chemistry	Building your first MD simulation; Exploring intermolecular forces; Energy in molecular systems; Chemical equilibrium and entropy in molecular systems; What does temperature measure? Discover Avogadro's Law; Under what conditions does the Ideal Gas Law apply? Colligative properties (vapor pressure lowering).
Biochemistry	Building your first MD simulation; Exploring intermolecular forces; Energy in molecular systems; Chemical equilibrium and entropy in molecular systems; Osmosis and osmotic pressure; Protein folding; Enzyme active sites.
Nanotechnology	Building your first MD simulation; Exploring intermolecular forces; Energy in molecular systems; Electrostatic self-assembly; Nanomachines.

The details for a few selected units are described below:

- **Building Your First Molecular Dynamics Simulation**

Students often conflate animations and simulations. It is important when introducing simulations to carefully explain, through examples, how simulations differ from animations. We have found that adequate explanation of the differences is crucial for students' conceptual development prior to working with simulations. This unit will introduce the basic features of MD simulations by guiding students to build simulations of gases, liquids, and solids. The goal is to learn the differences in behavior of molecules forming these states and the factors responsible for phase change. Students will learn how to add particles to a model (one at a time or many at a time). They will learn that heating and cooling the particles change their motions and these motions can result in changes of state: freezing, melting, condensation, boiling, and sublimation. They will learn to add gravity to cause liquids or solids to precipitate downwards. By contrast, in the gaseous state, molecules always fill all the available space. An important idea revealed by simulations, is that the sizes of the molecules themselves do not change when liquids turn into gases, even though they occupy a much larger volume.

This unit will introduce the technique of *comparative simulation*—the use of two models, side-by-side on the screen, that are identical in all respects except for one variable that students vary in one of the models while keeping the other unchanged (Figure 3). By comparing the unchanged *control model* with the *experimental model*, students have a powerful way to investigate the effect of one variable at a time[2].

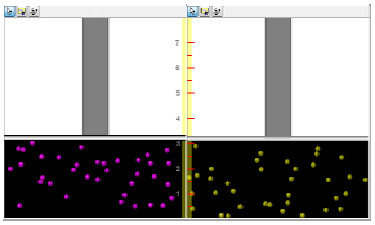


Figure 3. Comparative simulation: Two identical model containers are set up on an MW page to allow students to vary one and compare two simulations side by side.

- **Exploring Intermolecular Forces**

Understanding the physical origin of structural change, pattern formation, and system dynamics is difficult for most students. In this unit, students will explore intermolecular forces, including van der Waals, electrostatic, chemical polarity, and hydrogen bonding, and their effects on determining various macroscopic properties. To illustrate the universality of chemical forces responsible for many forms and functions, as highlighted by Feynman, the unit will cover concepts across subjects and leave the emphasis

[2] In his Foreword for a report on inquiry-based learning (National Research Council, 2000), Bruce Alberts singled out an inquiry skill: "One skill that all students should acquire through their science education is the ability to conduct an investigation where they keep everything else constant while changing a single variable. This ability provides a powerful general strategy for solving many problems encountered in the workplace and in everyday life."

of certain concepts to the instructor. For example, in general chemistry, students will explore how melting and boiling temperatures depend on the strengths of intermolecular forces to better understand why some substances are liquid or solid at room temperature, while others are gases. Biochemistry students will focus on hydrogen bonding and hydrophobic interactions. They will also learn to create positive and negative ions and observe how ions arrange themselves to minimize the electrical potential energy.

- **Energy in Molecular Systems**

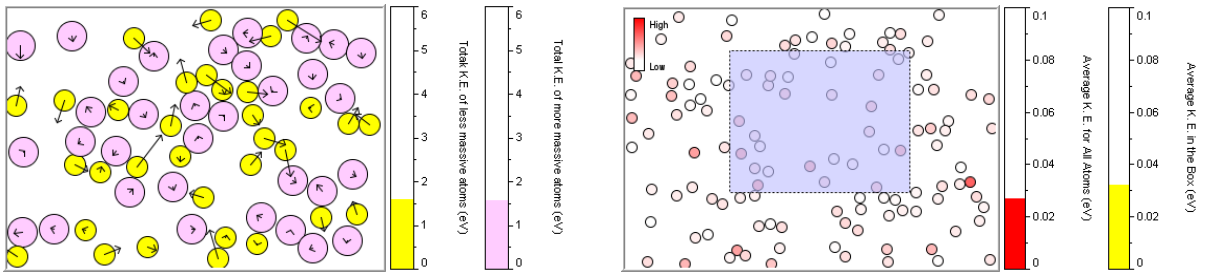
Like force, energy is a fundamental concept across chemistry. Over years of experience in teaching chemistry, however, we find that most students conflate force with energy and have great difficulty understanding the notion of negative potential energy associated with chemical bonding. This unit is designed to dispel common misconceptions related to energy in molecular systems (Galley, 2004). The exploration will start with a series of guided experiments to help students understand how the electrical potential energy and the Coulomb force depend on the relative positions of charged particles. By running the simulation and displaying the energy in a graph, students will see how potential and kinetic energy interconvert during elastic collisions. Once students understand the difference between energy and force, they will be challenged to design a device to store electrical energy. In a physical chemistry class, students will design a voltaic cell. In a biochemistry class, students will create simulations to explore the Gibbs-Donnan effect and how it produces electrical potential across biological cell membranes.

- **Chemical Equilibrium and Entropy in Molecular Systems**

MD simulation provides an effective visualization tool for addressing common misconceptions regarding the dynamic nature of chemical equilibrium. For many students, conventional static representations presented in textbooks are not adequate for making these ideas clear and they believe that at equilibrium, molecules stop reacting (Chiu, Chou, & Liu, 2002; Thomas & Schwenz, 1998; van Driel, 2002). In this unit, the illustrative power of MD simulation will help students learn the concepts of dynamic equilibrium in a variety of phenomena, including thermal conduction, phase change, chemical reactions, solubility of solids, and diffusion across barriers. Once they run various simulations of equilibria, they will be challenged with the inverse problem: Designing methods that prevent systems from equilibration. The difficult but important concept of entropy will be introduced in this unit.[3]

- **The Nature of Temperature**

A key concept for students to learn in first-year chemistry is that above absolute zero, all molecules are constantly in motion and it is the average kinetic energy—not the average speed or the average force—of



(a) (b)

Figure 4. Two simulations that show why the average kinetic energy is a good measurement of temperature. (a) This simulation shows that the average kinetic energies of two different types of particles adequately mixed in an equilibrium system are statistically identical. (b) This simulation shows that the average kinetic energy of the particles inside the selected rectangle, regardless of its size and location, is statistically equal to that of all the particles. In both cases, the bar graphs display the average kinetic energies of the sets of particles being compared.

[3] http://molecularmodelingbasics.blogspot.com/2010/03/illustrating-entropy.html

molecules that is linearly proportional to temperature. Some may remember this, usually by rote, but most do not realize that this means that more massive molecules have lower average speeds in equilibrium. This unit addresses the microscopic nature of temperature. Students will be challenged to create simulations to determine which quantity is proportional to temperature and why (Figure 4). Instructions will be provided on how to change molecular mass. Hints will be given on how to set up systems comprising two or more types of particles of different masses. Students will learn how to use MW's graphing tools to calculate and show average quantities, including average velocities and average kinetic energies.

- **Discovering Avogadro's Law**

In this unit, students will use the comparative simulation technique to discover Avogadro's Law—that equal numbers of gas particles at the same temperature and pressure occupy identical volume, regardless of their masses. Students will learn how to use a movable barrier to create an airtight piston. A constant force directed toward the particles can be imposed on the piston to apply constant pressure to the gas. Students will learn how to make the particles small and their intermolecular attractions weak to approximately simulate the ideal gas. They will learn how to adjust the temperature and pressure to change the volume of the gas. To explore Avogadro's Law, students will build two identical, side-by-side simulations of a gas under a piston, as shown in Figure 3. The two models have the same number of particles and all particles have the same size. Students will vary the mass of the particles in one of the simulations to discover that even large changes in mass, causing pronounced changes in the average molecular speeds, do not affect the volume occupied by the gas, as long as pressure and temperature are kept constant. As part of this unit, students will also explore the effect of changing the temperature or external pressure for one of the models. Before making each change, students will be asked to predict the effect on the relative volume when the temperature or pressure is changed and provide their reasoning. This level of detail will give researchers adequate data for assessing students' prior understanding. Then students will make the changes and report the results. Finally, they will reflect on whether their predictions were correct and, if not, how they would revise their reasoning, based on the simulations they have carried out. This unit has been tested in a one-semester physical chemistry course in 2009 but not in general chemistry, where we expect it to have a significant impact on student learning about gases.

- **Under What Conditions Does the Ideal Gas Law Apply?**

The Ideal Gas Law is usually covered in the first semester of introductory college chemistry. In this unit, the comparative simulation method will be used to investigate the conditions under which real gas behavior deviates from the Ideal Gas Law. The control model has small, non-interacting particles that simulate an ideal gas. This unit involves systematically changing the particle parameters including molecular mass, size, and strength of attraction, one at a time in the experimental model to see how they affect the volume occupied by the gas relative to the control model. For example, students will explore the effect of molecular size. By substantially increasing the size of the gas particles in the experimental model, students will observe an increase in the volume of the gas. Students will be guided to reason about what the increase in volume means. They can measure the change in the volume and relate that to the change in excluded volume of the molecules by geometrical calculations. Advanced students will be introduced to the complete van der Waals equation of state and how it better describes the behavior of a real gas.

Student Modeling Projects

Students will be provided with suggested modeling projects that provide opportunities to apply basic principles they have studied to explore more advanced phenomena or design useful devices. Suggested projects will include a theoretical introduction and hints on how to get started building a model. For each project, the teacher's guide will include a list of difficulties students may encounter and descriptions of advanced techniques they can use to solve them.

- **Projects for general chemistry** include, but are not limited to: 1) What is the origin of latent heat in phase changes? 2) What factors determine whether a reaction is endothermic or exothermic? 3) What is the effect of a catalyst on the activation energy and on the position of equilibrium of a reaction? 4) What is the nature of explosive reactions such as observed between hydrogen and oxygen? 5) Construct a device to separate molecules that differ in some property (e.g., boiling points, mass, electrical charge, etc.). 6) Explore the effects of magnetic fields on moving ions and apply what you learn to build a device to measure molecular masses (i.e., a mass spectrometer).

- **Projects for physical chemistry** include, but are not limited to: 1) Build a heat exchanger to efficiently conduct heat from a hot object to a cold object or an insulative barrier to prevent heat conduction. 2) Build a molecular model of a voltaic cell, an electrolytic cell, or a hydrogen fuel cell. 3) What is the origin of osmotic pressure? Build a simulation to demonstrate osmotic pressure or alternatively a device for desalination based on reverse osmosis. 4) How does capillary gas chromatography work? Build a molecular model of a gas chromatography column to separate two types of molecules that differ in mass and affinity for the column walls.

- **Projects for biochemistry** include, but are not limited to: 1) Explore the nature of hydrophobic interactions. 2) Design a polymer that folds into a unique conformation using combinations of hydrophobic, covalent, and electrostatic interactions. 3) How does ion exchange chromatography work? Build a molecular model of an ion-exchange column that separates molecules depending on their electrical charge. 4) Build a model illustrating separation of proteins by electrophoresis. 5) Explore the nature of osmotic forces that develop across semi-permeable barriers (like cell membranes). 6) Explore the origin of Gibbs-Donnan equilibria and how they affect cell membrane potentials.

- **Projects for nanotechnology** include, but are not limited to: 1) Build a model of the ion implantation technique. 2) Build a model of crystal growth based on atomic layer deposition. 3) Build a model that simulates sputtering and explore how to increase the sputtering yield. 4) Build a simulation that shows how to produce graphenes using Scotch tape.

The details for two modeling projects that were pilot tested at BGSU in 2009 are described below:

- **Designing an Apparatus to Separate Two Substances**

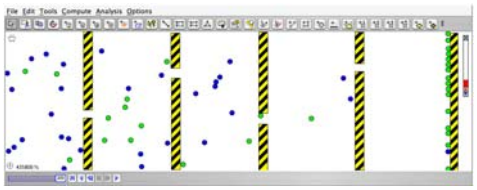


Figure 5. A multi-stage effusion device designed by a BGSU student to separate two substances.

The rules of this modeling project are: 1) The properties of the molecules cannot be changed; 2) The molecules cannot be moved manually; 3) The temperature can be changed; 4) An exaggerated gravitational field can be introduced if desired; 5) Any arrangement of static barriers can be introduced to restrict or guide the thermal motion of the molecules. The goal is to achieve as complete a separation of the two types of molecules as possible. Students devised a variety of solutions (see Fig. 5 for an example). For instance, some discovered how to change the properties of a barrier so that particles colliding with it will "stick" to its surface, simulating adsorption to a cold surface.

- **Designing an Energy-Efficient Window**

In this modeling project, students are challenged to solve a practical problem—how to prevent heat transfer, for example, through windows in buildings when the inside and outside are at different temperatures. Students are presented with an initial model that consists of a cold gas in the left compartment and a hot gas in the right one (Figure 6), representing the outside and inside of a building. The "window" is modeled with molecules having strong intermolecular forces and artificial restraints to keep them in place. Students run the provided simulation and find that the average kinetic energy of the molecules on the right gradually decreases while the average kinetic energy of molecules on the left gradually increases.

The simulation makes evident to the students the role of the solid barrier ("window") in transmitting the momentum and kinetic energy changes through collisions. Students are then challenged to modify the barrier in any way they wish to slow down the transfer of thermal energy, in other words, to create an insulating barrier. The design rules are: 1) No changes are allowed to the number and properties of the gas molecules; 2) The barrier must be constructed of individual particles, but their properties can be changed as desired (mass, size, number, disposition, intermolecular forces, etc.). During the 2009 test, several students emailed the instructor during the exercise asking whether an additional barrier could be introduced. As this was permitted, all students were subsequently informed. Interestingly, several students independently concluded through construction and testing that the best insulation could be achieved by using two barriers (double paned) and creating a vacuum between the barriers. This led to a discussion of how this idea is used to create highly insulating containers for storing cryogenic liquids, but that it would be impractical for windows. Since some material had to be placed between the two barriers, students had to determine what the best choice for the material should be in order to minimize heat transfer. In subsequent experiments, students explored gases of different masses and concluded that the heavier the gas, the better its insulating properties, given that the same number of particles would be needed to maintain constant pressure (which they learned from the unit about Avogadro's Law). This led to a discussion of the use of heavier noble gases in energy-efficient windows, available on the market.

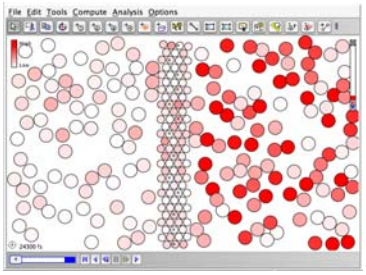


Figure 6. The initial setup of the heat transfer simulation. The molecules are colored by their kinetic energies: the redder the molecule, the greater its kinetic energy.

THE SOFTWARE IMPROVEMENT PLAN

The authoring environment of MW was originally designed for curriculum developers, not for use by average students. Therefore, despite the initial success with college students at multiple institutions, it is essential to make the authoring tools of MW easier to use for this project to succeed. The graphical user interface (GUI), which was developed based on Windows XP and earlier Mac OS X, will also be updated to meet the standards of newer operating systems. Key to this project, we will add new functionalities to accelerate model construction and make the construction process more intuitive and automatic. The new features will include, but are not limited to:

- **Copy and paste across models**. Students will be able to copy a part of a model and paste into another. This will allow them to quickly assemble a new model based on functioning parts of existing ones.
- **Develop smarter GUI**. Currently, efficient model construction can be done using scripts, which are flexible and fast but require significant time to master and debug. A smarter GUI will enable students to build models more efficiently without having to write scripts.
- **Improve analytic tools**. To see trends in chemical dynamics or evaluate the effects of different variables, students should be able to conveniently save and combine data from multiple runs and compare them in a single graph. We will add functionality to support these common analysis tasks.
- **Enhance computational engines**. Some advanced topics will require additions of new mechanisms and algorithms to the existing molecular dynamics and quantum dynamics engines in MW.

THE EDUCATIONAL RESEARCH PLAN

The goal of the research is to determine how the proposed "Constructive Chemistry" curriculum can be used in diverse settings to achieve greater success as we have seen in the preliminary research at BGSU. The research questions are: 1) Do students learn the science content with the units? 2) Do students learn modeling skills? 3) Is there any correlation between science learning and modeling skills? 4) What as-

pects of the constructive curriculum are most effective? 5) What implementation factors affect student learning? 6) What are teachers' and students' attitudes toward constructing models to solve problems?

Due to the exploratory nature of this project, we will adopt the design-based research framework, which is a paradigm for the study of learning in context through the systematic design and study of instructional strategies and tools (The Design-Based Research Collective, 2003; Walker, 2011). As the proposed instructional approach involves a complicated cognitive process in which students design models using sophisticated software, the research will be primarily qualitative in this phase. It will focus on analyzing students' models and design rationales, supplemented with case studies and student interviews for providing detailed process data. Pre/post tests and model scoring rubrics will be developed and used to quantify learning gains, modeling skills, and attitude changes. A complete list of data sources comprises:

- **Student models**. A model created by a student contains rich information about his/her reasoning process. It reflects the level of understanding of core concepts and the modeling skill of the designer. The diversity, variety, and creativity of students' models provide an ideal measure for the validity of the constructive approach. Based on the Knowledge Integration assessment framework (Linn & Eylon, 2011; Liu, Lee, & Linn, 2011), we will develop a model rubric for scoring students' ability to integrate and apply science concepts and their modeling skills to design solutions. In all measures, two independent evaluators will review models and score them in order to increase inter-rater reliability.

- **Embedded questions**. Students' answers to questions embedded in a curriculum unit provide additional sources to understand their motivations, reasoning processes, and analyses.

- **Design rationale**. Students will be required to present the design rationales for their models in their reports, which summarize their decisions, reasoning, and findings.

- **Screen recording**. We will use screen recording and usability test software such as *Silverback* to capture students' design processes and their interactions with our software. These videos will provide invaluable information for us to understand students' work and improve our software.

- **Survey and pre/post-tests**. The project will develop pre/post-tests that will be administered to measure the impact of the project on student learning, as well as student attitudes toward chemistry and modeling. A short survey will be developed to collect demographic data, prior academic achievement, prior science knowledge, mathematical skill, and prior experience with computer modeling.

- **Interviews**. The team will conduct interviews with randomly selected students. Interview protocols will be created and rubrics will be developed for analysis of the interviews. We will use prompts to elicit information pertinent to research questions such as these: What scientific concepts did students master sufficiently to apply appropriately in new contexts? Which conceptual misunderstandings persist? We will also ask students to describe the strategies they used to build their own models and how they dealt with challenges and difficulties. Did they encounter unnecessary frustrations that can be addressed with program fixes? These interviews will help us examine what and how students learned.

THE DISSEMINATION PLAN

The team will disseminate "Constructive Chemistry" through the National Science Digital Library (NSDL), which is a partner of CC in a current project (www.concord.org/projects/concord-consortium-collection), and the Northwest Ohio Center of Excellence in Science and Mathematics Education (COSMOS) (cosmos.bgsu.edu), with which the BGSU team is involved (see letter from Prof. Midden, Director of COSMOS). The PI at DCTC leads the Nano-Link regional network that promotes nanotechnology education at multiple grade levels by providing comprehensive educational resources. Nano-Link will disseminate the project materials through its hands-on educator workshops and classes. The team will also present the project results through conferences and journals.

PROJECT EVALUATION

The project will rely on the expertise of the Advisory Board for external evaluation of the project. The evaluation will focus on these criteria: 1) How well the project meets the stated goals of improving the technology. 2) The scientific accuracy of the content of "Constructive Chemistry" instructional materials. 3) The effectiveness of the instructional materials in promoting deep conceptual learning. 4) The appropriateness of the review and assessment strategies. 5) The ease with which instructors are able to use the technology and the curriculum materials. 6) Changes in attitudes of students from diverse backgrounds towards learning about chemistry using "Constructive Chemistry." In addition, the Advisory Board will help identify which components need further improvement. The advisors will meet in a closed session to review the project materials and results during the annual meetings. They will produce reports with recommendations for project staff that will also be forwarded to the cognizant NSF program officer.

PROJECT SCHEDULE

The project comprises cycles for technology and instructional materials development, classroom tests, educational research, and dissemination phased over two years, as follows. **January 1, 2013-December 31, 2013:** The team will develop the "Constructive Chemistry" materials and pilot-test them at BGSU and DCTC. The initial version will be developed in the first six months. The software developer will work closely with the curriculum developers to add new software capacities required for the units. Instruments such as student surveys, pre/post-tests, and embedded assessments will be devised to gauge student learning. In the summer, participating instructors from BGSU and DCTC will hold a workshop to learn about the software, the curriculum units, the constructive pedagogy, and the research methodology to assess student creations. The field tests are scheduled to begin in the fall. All students will be surveyed to collect their background data. The Advisory Board will meet at the end of the year after preliminary results are obtained. **January 1, 2014-December 31, 2014:** More classroom testing and implementation will occur in this year. Materials and software will continue to be improved. Student data analysis and interviews will be conducted. We will disseminate our materials as described in the Dissemination Plan above.

PROJECT PERSONNEL

The Advisory Board

The project will be advised by a group of outstanding chemistry professors who have agreed to meet with the project staff once a year to formally evaluate the project.

- **Dr. Renee Cole** is Professor of Chemistry at the University of Iowa. Her research covers the impact of visualization and computation activities on student learning and development. She will bring her research experience to guide this project.
- **Dr. Thomas Holme** is Professor of Chemistry at Iowa State University. His combined expertise in both chemistry education research and computational chemistry will be an important source of inspiration for this project.
- **Dr. Hannah Sevian** is Professor in the Curriculum & Instruction and Chemistry Departments at the University of Massachusetts, Boston. A theoretical physical chemist and a chemistry education researcher who is dedicated to the education of underprivileged students in urban communities, she will ensure that this project will produce materials of the highest quality suitable for all students.
- **Dr. Dunwei Wang** is Professor of Chemistry at Boston College. His research focuses on understanding the science of energy conversion and storage. He is excited about the applications of new technologies in promoting undergraduate teaching and will advise us on student modeling projects.

Staff at Bowling Green State University

- **Dr. Neocles Leontis,** Professor of Chemistry at BGSU, will serve as the PI at BGSU and will have overall responsibility for the research and development of the project. He holds a Ph.D. in biophysical chemistry from Yale University. He has taught chemistry at both undergraduate and graduate levels, including general chemistry, physical chemistry, biochemistry, and bioinformatics. He is an NIH/NSF-funded researcher whose primary research interests are RNA structural bioinformatics, molecular modeling and simulation, and nanotechnology. He is very active at BGSU in promoting educational innovations that improve student conceptual learning at all levels. In collaboration with faculty across the university, he recently founded the BGSU Innovative Teaching Group to disseminate evidence-based teaching innovations university-wide.

- **Dr. Andrew T. Torelli**, Assistant Professor of Chemistry at BGSU, will serve as Co-PI. He is trained in macromolecular X-ray crystallography and, since coming to BGSU, has actively participated in multiple opportunities to improve the efficacy of his teaching. He is an active member of the BGSU Faculty Learning Community for increasing student learning through strategic assessment in STEM education and has worked with a local high school to introduce students to X-ray diffraction.

- **Dr. Peter M. Blass**, Instructor of Chemistry at BGSU, specializes in undergraduate education, especially first-year students. He holds a Ph.D. in chemical physics from the University of Texas at Austin. He is a member of the BGSU Innovative Teaching Group on campus and works on development of online material for general chemistry courses. In the general chemistry program, he has promoted peer-to-peer and mentor-led teaching to significant effect.

- **Dr. David Erickson**, Instructor of Chemistry at BGSU, teaches primarily introductory chemistry and forensic science courses. He holds a Ph.D. in analytical chemistry from Purdue University. His focus continues to be on implementing new strategies for learning in and out of the classroom. David also applies new educational technologies in his classes.

Staff at the Concord Consortium

- **Dr. Charles Xie** will serve as the PI at CC. He has 12 years of research and development experience in STEM education. He is the primary author of eight papers in peer-reviewed journals in science and engineering education, including a recent cover article in the *Journal of Chemical Education* on infrared imaging. As the creator of the award-winning *Molecular Workbench* software, he will be responsible for enhancing its functionality to ensure the success of this project. Additionally, he will facilitate the educational research part of this project. Charles holds a Ph.D. in materials science and engineering from the University of Science and Technology, Beijing.

Staff at Dakota County Technical College

- **Deb Newberry** will serve as the PI at DCTC. She currently serves as the Director and PI for Nano-Link and is the lead faculty for the Nanoscience Technology program at DCTC. She is a trained nuclear physicist who spent 23 years in the corporate world performing radiation analysis on satellite systems and serving in executive management. She is the co-author of the recent book, *The Next Big Thing is Really Small: How Nanotechnology Will Impact the Future of Business*. She has been responsible for the organization and content of the courses for the Nanoscience Technology program at DCTC. She will collaborate with BGSU and CC to integrate "Constructive Chemistry" into the DCTC nanotechnology courses and the Nano-Link Resources Center.

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