Computational Chemistry
Training for Teachers
Summer 2007

Detailed Program Description
I. Abstract

The purpose of this project is to enhance teachers’ and students’ content knowledge by engaging teachers and high-school students in the solution of unique scientific problems that will be of publishable quality (developing specialized science literacy as called for in national science standards). As national science standards indicate, science is a very practical endeavor that involves sophisticated and complex ideas and methods, which are learned best through experience – by doing it. In recent years, institutions of higher learning have been aggressively implementing new pedagogical approaches that emphasize inquiry. The purpose is for labs to have less of a “cookbook flavor” to them, and for students to learn concepts in the process of experimenting. These new approaches put science students a step closer to “doing science,” rather than merely “learning about science.” Nevertheless, in order to cover the appropriate content necessary for a well-rounded science education, experiments in teaching labs are usually designed to follow the “discovery” format; the expected outcomes are well known by the instructor. Part of what excites young minds about science is facing the unexpected, and having to explain it, or discovering something that was previously unknown. Working on an authentic research project is the ultimate model for an inquiry approach to learning science. In this model, mentors and students work together to obtain data, interpret results, and develop new solutions to unique scientific problems.

The proposed project aims at helping chemistry teachers to use modern tools of computational chemistry to solve scientific problems, and equipping them to use those tools for discovery experiments in high school classes. Additionally, it is a goal of this project to train teachers to mentor students as they work on scientific projects. A third goal is to inspire students, particularly women and other underrepresented groups, to pursue an education and career in science by giving them a vision of what can be accomplished through science, exposing them to the excitement of scientific presentations and inquiry, and providing them with direct contact with the scientific community.
II. Project Summary

The Rhode Island College Physical Sciences Department, RIC’s Feinstein School of Education and Human Development, and Providence Public School District will implement a program whereby high school teachers and students participate in inquiry activities in inorganic, physical and biological chemistry, using computational chemistry as the main tool. Teachers will be trained to use computational chemistry to implement inquiry experiments at the high school level. Teachers and students content knowledge and scientific literacy will be enhanced through authentic investigative experiences, and all participants will present their findings in a local symposium and in an international conference in computational chemistry. The goals of this program are to better equip teachers to instruct and mentor students using scientific discovery, to provide a scientific research and inquiry experience for teachers, and to expose students to the wonders and excitement of scientific discovery, thus increasing their enthusiasm and improving recruitment and retention of science students.
III. Narrative

A. Statement of Need

Science and technology are central to our modern society, which relies on scientific developments to meet needs ranging from health to communication and transportation. Science also helps us fulfill a natural yearning to understand who we are, and how nature functions. It is therefore unacceptable that Rhode Island students are insufficiently knowledgeable about science and generally lack the necessary preparation to enter careers in science and engineering. As indicated in the 2006 report of the PK-16 Advisory Committee on Science,¹ this unfortunate observation has been independently made by many groups such as Achieve Inc., The Education Trust, the Thomas B. Fordham Foundation, the Business Roundtable, the United States Chamber of Commerce, and the Rhode Island Governor’s Blue Ribbon Panel on Mathematics and Science Education. Given the dynamic and empirical nature of science, much of the skills and content of science necessary to improve education in Rhode Island are best learned through hands-on inquiry and discovery approaches. With that line of thought, the aforementioned committee made several specific recommendations that were carefully summarized into five main recommendations. Three of them are directly addressed in this proposal: 1) Students must demonstrate the skills used in the process of science, 2) Students must have authentic investigative experiences, and 3) Professional development and pre-service training for science teachers must emphasize instruction in pedagogy, content, and experimental investigation.

The importance of laboratory and field-work experience in science is such, that the committee strongly recommended a significant increase in the time high school students invest in those activities, so that science courses should devote a minimum of 40% of their time in those activities. New ideas and methods are needed to present content through laboratories and investigative experiences, and according to B. S. Bloom,² just like in science itself, developments in science education should be the result of systematically testing models and hypotheses. D. S. Domin nicely summarizes several models that have been tested for laboratory and field-work experiences.³ There are four main models in use in recent years: the expository, the problem-based, the discovery, and the inquiry approaches. The expository approach is the most traditional

¹ PK-16 Advisory Committee on Science to PK-16 Council of Rhode Island, PK-16 Advisory Committee on Science Report and Recommendations, 2006. Available at http://www.ribghe.org/sciencereport06.pdf
approach (which resembles the use of a cookbook), where procedures are given to students, deductive thinking is used, and the outcome is predetermined. The problem-based approach also uses deductive thinking and has predetermined outcomes, but rather than using prepared procedures, it uses questions to prompt students to develop a procedure. The discovery approach uses prepared procedures to reach predetermined outcomes, but inductive thinking is used. This approach is also called guided-inquiry, and the great majority of projects that claim to use “inquiry” are actually in this category. As in discovery, the approach that is most appropriately called inquiry uses inductive thinking, but procedures are not pre-assigned. The most important characteristic of inquiry projects is that unlike all the other approaches, the outcome is undetermined. That is exactly what happens in cutting edge science. Clearly, the ultimate “inquiry model” is to expose students to actual scientific research projects – nothing can be better described as an “authentic investigative experience” than that.

The benefits of engaging high-school students and college students in research have been touted by the National Science Foundation, the American Chemical Society, and Council on Undergraduate Research; nevertheless, that idea is not widely implemented in science for several practical reasons, including the long-term nature of most research projects and the inaccessibility to the expensive equipment that is typical to cutting edge research. Those difficulties are easily overcome in the field of computational chemistry, where short-term projects can be developed relatively easily, and the cost is minimal compared to other fields of research. Accessibility to inexpensive scientific software also makes it possible for high school teachers to implement inquiry projects with their own students during the academic year. Additionally, the use of computers and exposure to technology are natural to the field.

The whole field of theoretical physical chemistry was developed as a natural offspring of the developments of modern physics in the first half of the 20th century. The development of relativistic and non-relativistic quantum mechanics served to explain important experiments in chemistry, and to generate predictive models in all fields of chemistry, physics and molecular biology, yet the powerful equations of quantum mechanics are not solvable analytically. It was not until the advent of computers that pioneers such as Henry Shaffer and Nobel laureate John Pople started developing approximate solutions to the Schröedinger equation in the 1960’s, and since then models have matured to the point that theoretical chemistry has become crucial to

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modern research in chemistry. Not only quantum based models, but models based on classical physics are used today, and several areas of research have increased productivity due to the facility with which predictions and new ideas are accurately tested in silico. For example, the average time for new drug discovery is fourteen years, but the use of computer models can reduce it to as little as three years. To a large extent, the community of developers of new theories remains relatively small, but readily available software has enabled the implementation and wide use of new theories by a much larger community of users. For example, some of our own theories and methods are included in the most widely used commercial software in the field of chemistry. Although theoretical chemistry remains one of the most intense uses of supercomputer time, new methods and faster workstations contribute to the widespread use of predictive computer models. The use of existing models to solve chemical problems (as opposed to the development of new methods) is usually called “computational chemistry” (rather than “theoretical chemistry”). Training in computational chemistry is a necessary component in the education of the next generation of chemists, and modern programs in chemical education implement components of computational chemistry in practically all lab courses, as is the case at Rhode Island College. There is no reason why this very accessible type of technology should not be used at the high school level. Hamilton College, one of our partners in the Molecular Education and Research Consortium in Undergraduate computational chemistry (MERCURY) consortium has already successfully engaged high students in computational chemistry research, and greatly improved their recruitment to science, and to chemistry in particular. Here we not only propose to engage high school and college students, but also teachers, who will be equipped to mentor students and use new technology in their classrooms during the year.

Almost ten years ago, the Chemistry and Biochemistry and the Physics Departments at California State University at Fullerton created a Center for Molecular Structure, which successfully moved their mode of teaching from the “problem-solving approach”

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8 Gaussian 03, Frisch, M. J. et. al; Gaussian, Inc., Wallingford CT, 2004.
9 Recent methods developed in our lab allow for very accurate calculations to be reproduced 300 faster than previous methods, eliminating the need for supercomputers for certain calculations.
to more engaging methods using computer technology. In that case, computer graphics served for visual reinforcement and interpretation of concepts. Here we expect to go well beyond reinforcement, to offer predictions and explanations to experimental data, using accurate computer models.

In summary, this project intends to serve three groups of people in the educational system: science teachers, high-school students, and college students. Several of their needs are going to be addressed through this project:

1) The aforementioned groups typically have insufficient opportunities to participate in scientific developments. Lack of research experience typically leads to a misunderstanding of how science is done. There are fundamental differences between idealized models and practical approaches used in science. In practice, scientists use both deductive and inductive thinking, unlike the unidirectional “textbook” approach suggested by the “scientific method;” the intricacies of scientific thought are only learned through experience.

2) Science teachers need to be well equipped to use modern pedagogical approaches, which focus on inquiry, and they need to be prepared to use state-of-the-art computer technology (now central to scientific experimentation), which is currently accessible at the high-school level. Teachers who have experienced cutting-edge approaches and tools will be more knowledgeable and confident teachers of future scientists.

3) In order to better meet the economic needs of the state of Rhode Island, institutions of higher learning must increase recruitment and retention of science students. For that to be accomplished, interest in science, science content knowledge, and confidence in learning and in science must be fostered in students early in their academic careers, particularly among women and groups that are traditionally underrepresented in science.

B. Objectives and Expected Outcomes

The main objectives of this project as it relates to teachers are to use the tools of computational chemistry to equip teachers for scientific inquiry, to provide new tools and approaches for engaging high school students, and to reinforce and complement the content necessary to effectively teach high school chemistry. Regarding high school students, our goals are to expose them to the excitement of scientific discovery, increasing their knowledge base, and generating enthusiasm, which should increase the number of students choosing to pursue science. As to college students, they should reap similar benefits, but they should also gain the new experience of mentoring others.

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thus elucidating the challenges and personal fulfillment of teaching. More specifically, our goals as described in the alignment with GSE’s and other standards, are the following:

1) Teachers will take a two-week (3 credits) intense course in computational chemistry, focused on experiments and techniques for high school classrooms and labs. They will gain a descriptive and practical understanding of quantum mechanics, as it applies to atoms and molecules and will learn about the applications and physical underpinnings of computational models. They will learn how modern models use equations of motion to describe molecular behavior and collisions. It is expected that as a result of this course, teachers will be prepared to use computational chemistry in high school activities, particularly those that are inquiry based.

2) After the initial course, groups of teachers and students will be given a problem or a hypothesis in chemistry, biochemistry or physics, and will choose how to use computational chemistry to answer scientific questions. They will judge the appropriateness of the different computer models to elucidate the scientific problems at hand. After intermediate results are available they will develop new hypotheses, and predict outcomes. It is expected that participants will become more familiar with the scientific method and teachers will have a first-hand experience mentoring students through an inquiry-based project.

3) Teachers and students will obtain their results from computations, and compare them with experimental data and other published values from the scientific literature. Different groups will also discuss the results of their respective projects with each other, to assess their quality and significance, and to suggest further steps. It is expected that participants will become more proficient in team work that is now typical of scientific research groups, and will develop a sense of the peer-review process commonly used in science.

4) Participants will use results of scientific models to reach conclusions regarding the problems at hand, and will report their findings in writing. It is expected that they will improve their ability to organize ideas, data, and evidence, in order to reach reasonable conclusions.

5) Teachers and students will be exposed to the scientific literature and will attend seminars or workshops presented by leading scientists. They will discuss and share their results and conclusion in a local symposium, with input from science faculty from RIC, and at the end of the program they will present their results at an international conference. It is expected that participants will become familiar with common mechanisms to disseminate scientific knowledge, and will gain a better understanding of how individual projects contribute to the whole body of knowledge in science.
6) Participants are expected to increase their understanding of science content by studying several types of problems:

a. Teachers and students will analyze the relationship between structure and function in chemical and biological systems, by examining the effect of metal replacement on the structure and function of metalloproteins, evaluating equilibrium structures for weakly bonded clusters, examining structure-activity relationships in sugars, and exploring potential energy surfaces.

b. Teachers and students will consider and discuss energy in several projects involving thermodynamic cycles for isodesmic reactions, and will use thermochemical properties (including atomic properties) as a test for computational methods. They will also consider energy through evaluations of transition states, activation energies and rates of reaction.

c. Teachers and students will explore periodic trends in different systems comparing dispersive and hydrogen bonded systems, different chemical behavior in the first transition series in the periodic table, and covalent and ionic character in solids.

d. Participants will examine when it is possible and appropriate to use models based on classical physics, as opposed to quantum mechanics, by testing the extent to which electrostatics contribute to the total interaction and comparing classical models with quantum mechanical models.

Sample project descriptions are given in Appendix I.

C. Description of Activities

While the direct activities for this project are most intense during the summer, continual mentoring of teachers and inclusion of high school students in research is expected to continue during the year. The project is designed to ideally accommodate six teachers and six high school students the first year. A stipend will be provided to offset typical financial needs of high school students, who often work during the summer.

Preparation

In May, a group of three college students, with extensive experience and expertise in computational chemistry, will be introduced to the program. They will learn about the labs and scientific projects that will be used. It will be important for all the student-staff to be very familiar with the science behind all the projects. They will be trained in computer administration and will be instructed on how to help all the participants of the project. This training will last two weeks. Given the previous research and publication experience of these students, their role is crucial to the success of this
project. They will help teachers to get acquainted with computational chemistry, and later will work side-by-side with the teachers in mentoring high-school students. We expect the interaction between teachers and science students to be mutually beneficial.

**Computational Chemistry Course**

For two weeks in the beginning of the summer, teachers and college students will attend lectures and participate in hands-on activities (guided inquiry labs) with the purpose of developing intense familiarity with the methods and software utilized in computational chemistry research. There will be examples and suggestions on how to integrate computational chemistry into high school labs. The course content will include a descriptive background in quantum mechanics and modern computational methods, and will be directly linked to the GSE’s. Many of the traditional components of coursework will be completed during this phase, including reading, discussion and performance. During these two weeks, there will be a minimum of 42 contact hours, and teachers will receive three graduate credits for their participation. Participants will also receive personal copies of a book on computational chemistry, which will serve as a resource during the course, during the research activities, and during the year when new ideas are being implemented at the high schools.

**Research Projects**

After the initial coursework, teachers will become acquainted with the scientific problems that were developed in the spring. High school students will join the program, and the teachers and college students will participate in teaching them how to use the scientific software. Participants will be divided into small groups including teachers and students, and each group will be presented with an unique hypothesis or scientific problem that is presently of interest to research scientists. The scientific problems will be in the fields of biochemistry and biology (proteins), environmental sciences (atmospheric chemistry), solid-state physics (ionic and metallic solids), spectroscopy (microwave and IR), and theoretical chemistry (model comparisons). See Appendix I for samples. These research groups will be challenged to devise a plan to shed new light on the problem at hand. At that time, with the help of college students with research experience, teachers will mentor high school students through the process of choosing appropriate methods and approaching a problem as a scientist.

Participants will try their ideas, with the intent of truly contributing to the body of scientific knowledge. They will be asked to search and read some of the available scientific literature. When intermediate results are available, participants will have to
judge whether their data is useful and whether a new hypothesis needs to be developed. During the whole process, groups will be encouraged to discuss and compare their problems and results with other groups, offering suggestions to each other on how to successfully proceed through their scientific inquiry. Eventually, each group will be asked to write a summary of their activities, including conclusions about the scientific problem they handled. This activity is intended to offer first-hand experience in scientific discovery.

**Workshops and Seminars**

Starting in the second week, there will be a series of three or four invited speakers who will introduce program participants to different methods and applications of computational chemistry. High profile, successful scientists from well-known universities or companies will participate in this series. All program participants will benefit from these seminars, which will be open to the public.

**Symposium and Conference**

After their research activities, program participants will share their findings in a symposium format. Rhode Island College faculty and students, as well as other guests will be invited. Those in attendance, especially faculty, will be asked to assess the projects and presentations, filling evaluation forms and offering constructive criticism. This colloquium will serve as a preparation for an international conference (the MERCURY Conference in Computational Chemistry), in which some of the program participants will present their results. Participation in this conference will be crucial for the participants to be able to place their contributions into the greater context of the scientific community. Interaction with other scientists and science students will be important to elucidate the nature of scientific discovery. In Appendix II, an article written by RIC students sheds some light on the value of this experience.

**Planning and Implementation for the Academic Year**

After the conference, participants will be asked to assess all aspects of their experience in this program. Participating teachers and the project directors will plan a schedule for the mini workstations to be used by the different schools during the year, with the intent of implementing new activities at the high schools, involving the use of computational chemistry. During the academic year the program director will be in contact with participants and will be available to help them to implement learned concepts in their chemistry classes.