2005-2007 LITRE Grant Proposal

1. Project Title:

Computational Chemistry Laboratory II

2. Project Coordinator:

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3. Other Participants:

Computational Chemistry Committee
Staff Member
(individuals to be determined)

4. College or Unit:

Physical and Mathematical Science

5. Department:

Chemistry

6. Project Description:

Content for Computational Chemistry Laboratory II, a one-credit hour, sophomore-level laboratory course for inclusion within the chemistry curriculum, will be developed. This course is to complement Computational Chemistry Laboratory I which is currently in the testing phase.

Both courses are inquiry-driven and seek to equip our students with computational tools which are increasingly demanded in the marketplace. They furthermore are designed to enhance student understanding of chemistry at a molecular level but in a visual way with an emphasis on fundamental interactions and drawing upon skills learned in physics and mathematics.

The project will involve generating course content and figures suitable for web-delivery and constructing inquiry-guided exercises with commercially available software. Once developed, the course with one section of 12 or fewer students will be pilot tested and data will be collected and used in assessment. The course will then be edited and offered to all chemistry majors. The final phase of this project will be to disseminate the course to other universities.

7. Project Objectives:

7a) Goals and the Enhancement of Student Learning

To explain the goals of the course and the impact on student learning, it is helpful to describe more fully how the course is structured. This course is the second computer laboratory course in a two-semester sequence. The second course will primarily focus on quantum mechanical calculations. Starting with fundamental interactions between electrons and protons, the course will add a layer of mathematical and conceptual sophistication to the descriptive quantum theory taught in general chemistry. The course will then proceed to the construction of atomic and molecular orbitals which will be used to study bonding in chemical systems. The software which can perform these quantum mechanical calculations has the advantage of a small learning curve and is highly visual. Model systems will also be used and comparisons will be made to literature values. The examples in the latter portion of the course will be drawn from inorganic chemistry which complements the emphasis in the latter portion of Computational Chemistry I which uses organic chemistry examples.

To illustrate the connections between courses and the emphasis on computational models, please refer to the flow chart below of one laboratory exercise that will be developed. Each time the word compute is used, it refers to a quantum mechanical calculation which will be performed using a software package. All action words are underlined to illustrate the various types of activities the students will be expected to do and hence a place where there are opportunities for student assessment (both the students' reflections and the instructor's).

<please see email for figure>

Figure 1. Flow chart of a computational chemistry laboratory.

There will thus be an emphasis on inquiry-guided instruction, allowing students to discover a pattern or predict a result. Computational exercises are even more amenable to this discovery than traditional wet-lab experiments in that parameters can be manipulated with the computer (for example, a charge can be turned off), and the effect of that change seen, where such a manipulation cannot be done in experiment. Care will be taken to ensure the tightest coupling possible to the mathematical foundation of the calculations to avoid degeneration to black-box pedagogy.

As with the first course, the second course is an effort to add a layer of chemical and mathematical sophistication in between chemical concepts taught in the freshman and junior years. General chemistry introduces molecular orbital theory but it is highly descriptive since most students have not had a full year of calculus. In the junior year, this subject is revisited in physical chemistry, but in a highly abstract form. Meanwhile in the sophomore year, this theory is a very useful tool to illustrate organic chemistry reactions and it is also heavily used in the beginning of the junior year in inorganic chemistry. Thus a major goal of this course is to bridge these subjects and provide instruction in an area of chemistry which will give students a conceptual framework for understanding concepts in various sub disciplines in the chemical sciences, even beyond traditional organic or inorganic chemistry.

To summarize the course, there are five Course Content goals:
1. Understanding the forces that hold matter together
2. Graphing wavefunctions
3. Constructing molecular orbitals
4. Visualizing of molecular orbitals and bonding in inorganic systems
5. General use of scientific software packages

In addition to course content, there are five Curriculum goals. These goals were articulated already in the LITRE 2004 proposal and have not changed since this course is the companion to Computational Chemistry I.
1. To introduce computational chemistry/molecular modeling as a tool
2. To develop a physical framework of how energy relates to the geometrical arrangement of atoms in space and how this guides chemical reasoning.
3. To provide a foundation upon which more sophisticated problems can be assigned in later semesters that use these tools and software.
4. Chemistry is a mixture of quantitative and qualitative information yet our curriculum is frontloaded with qualitative courses. These labs will provide a balance in order to 1) acquaint students with the quantitative aspects of the discipline and 2) provide a step-wise introduction to those aspects.
5. To provide a ramp up to the physical chemistry sequence in the junior year, especially for those students who are less mathematically inclined and need an introduction that is more hands-on. In a computational chemistry course, the student will be able to visualize what an equation does in regard to a chemical system.

7b) Long term impact

Successful development, implementation, and assessment of this project will have an impact on the chemistry department in two areas. First, it gives undergraduates an introduction to an important area of chemistry that is used across many disciplines. It also provides a ramp up to the junior year where faculty teaching advanced courses can require students to work problems to which there are no analytic solutions. Thus, although just one course, its affects reach across the curriculum. Secondly, this course is likely to also impact both the undergraduate and graduate curriculum in that it is the beginning of an effort to integrate computational chemistry in all courses. Many graduate students also have a need to learn such computational skills.

This course along with its Computational Chemistry I counterpart represents a unique approach to integrating computational chemistry into the curriculum. NC State University can become a leader in the area of undergraduate computer-based learning in the chemical sciences should this course be successful. Key to this long-term impact will be successful assessment and dissemination.

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8. Estimated number of students affected:

An initial enrollment of 12 students will serve as a testing of the course. Once the initial assessment is complete and the course has been edited, a full class of 50-60 students will be enrolled every spring semester.

If the courses are successful and space is available, we plan to expand this course to other departments in related fields (chemical engineering, physics and biochemistry).

This project is also just the initial step toward integration of computational chemistry and computational chemistry tools in the majority of courses offered in the department.

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9. Outcomes of the Project:

The following list summarizes the impact this course is expected to have on student learning.

Students will:

1) Learn a major computational tool (a quantum mechanical method)
a)Set up and run a quantum mechanical calculation and interpret results
b)Learn the theory behind the calculation
c)Graph results
d)Visualize bonding in chemical systems
e)Develop a framework for understanding chemical systems from a computational viewpoint
2) Compare results from computation with experiment
3) Apply concepts from physics and math courses to chemical systems
4) Be able to solve more sophisticated problem sets in advanced courses

The example outlined in the flow chart in figure 1 succinctly illustrates how this course meets the four dimensions of the LITRE Goal 1:

a) Problem solving
Students will learn to set up a model to predict the amount of energy required to break a bond. To graphically represent this bond energy is a qualitative skill previously learned, but students would have no way of computing this value without such a model coupled with the selected computations.

b) Empirical inquiry
Students will be exploring the trends in energy when electrons are added or removed from neutral atoms. Only one of the two processes is amenable to computations and they will be able to discover it by comparing computed values to experimental ones.

c) Research from sources
Students must compare calculated results to experimental ones and evaluate the effectiveness of the computational method at reproducing those values.

d) Performance in the discipline.
Students will be doing fairly advanced computations, applying the physics and

calculus to the problems. To have students be able to perform at a higher level on Bloom’s Taxonomy requires course content be written in such a way that integrates these skills.

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10. Project impact on NCSU:

Successful development, implementation and assessment of this project will have an impact on the chemistry department and NCSU. This course is a major step toward modernizing the chemistry curriculum since these tools are widely used in industry and academia in all disciplines of the chemical sciences.

Since this course along with the Computational Chemistry I counterpart represents a unique approach to integrating computational chemistry into the curriculum, NC State University can become a leader in the area of undergraduate computer-based learning in the chemical sciences.

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11. Project Assessment Plan:

There are several types of assessments to ensure learning outcomes are met:

• Pre-testing students on concepts that are learned in previous courses and used again in this course to establish the baseline of knowledge.
• Checkpoints will be taken the first time the course is tested to see how quickly and correctly students proceed through each laboratory. This information will be important in order to later edit lab content, length and difficulty level.
• Performance on class assignments and exams. All classwork and homework assignments will be handled through webassign. (This will be the primary assessment tool to monitor progress towards the outcomes listed in #1 above in section #9.)
• Performance in later courses, especially in assignments that use the same software used in this course. A survey instrument will be made available to instructors in subsequent courses.
• For affective assessment, end of course evaluations.

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12. Staffing and Support:

Laura Sremaniak: Coordinator of project who will write the course material, choose appropriate software and integrate the material with the software

Programmer who will generate figures, tables and make material suitable for web-based delivery.

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13. Financial Support Requested:

EPA salary total: 3000.00
SPA salary total: 2500.00
Other salary: 0
Equipment: 3500.00

Cost associated with assessment: 0
Other financial support requested: 1000.00
Total Funds requested: 10 000.00
Additional Explanation of how funds will be used:

EPA salary: $3000.00 for a portion of summer salary for assessment and editing of the course, writing advanced problem sets that use the software students learn in this course
SPA salary: $2500.00 for a programmer to generate figures/graphs in the electronic text.
Other salary: n/a
Equipment: $3500.00 for an additional 8 copies of software. The department is seeking to teach these sections in groups of 25. We currently have a room of 12 computers but the student traffic in that room is such that it will not be sufficient to accommodate the students in this course doing homework exercises. For technical reasons, this software was not able to be put on the PAMS computing realm.
Cost associated with Assessment: n/a
Other (Travel): $1000.00 It is desirable that this course be disseminated and also to get feedback from outside faculty from other universities which such settings provide.

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14. Funding Breakdown:

Total funding requested for fiscal year 2005-2006: 10 000.00
Total funding requested for fiscal year 2006-2007:

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15. Staff Support and/or Technical Support Requested:

n/a

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16. Timetable for Implementation:

Computational Chemistry Course content will be tested in Spring 2006. (Figures will be added on a weekly basis.)
June 2006: Assessment of both courses will be performed. Both courses will be edited.
July 2006: Attend Biennial Conference in Chemical Education. Purchase additional software.(This could be shifted to a conference in 2007.)
Aug 2006-May 2007: scale up to class of 60. Continue Assessment.

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17. Human Subjects Protection:

If your proposal project involves research using human subjects, you will need approval from the Institutional Review Board for the Protection of Human Subjects in Research (IRB) prior to final approval. IRB information is available at http://www.ncsu.edu/sparcs/irb

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18. Proposal Release:

By submitting this proposal the applicant grants the LITRE Advisory Board permission to make this proposal available as an example for future grant applicants. All personal information will be removed if this proposal is used as an example.

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