

Division of Academic Affairs
Technology Fee – Project Proposal
2016

Proposal Deadline: Friday, January 22, 2016

Project Proposal Type

Instructional Technology Enhancement Project (ITEP)

Focused projects proposed by an individual or small team with the intention of exploring new applications of instructional technology. ITEPs will typically be led by a faculty “principal investigator.” ITEPs are time-limited projects (up to two years in length) and allocations of Technology Fee funds to these projects are non-recurring.

Project Title

PC Spartan for Computational Chemistry

Total Amount of Funding Requested

\$12,300.00

Primary Project Coordinator

Dr. Christopher Nicholson, Assistant Professor of Chemistry

PC Spartan for Computational Chemistry

1. Project Description

Modern chemistry, both academic and industrial, relies heavily on an ability to merge computational skills with traditional laboratory techniques and analysis. From the ability to assess molecular shape and interactions to the ability to model reactions and predict outcomes, no field of chemistry is untouched by modern computational methods. For many years a rudimentary program, PCModel, was used for very simple calculations and analyses. Unfortunately the capability of PCModel has long been surpassed by programs which are designed for use by students as low as high school and introductory college chemistry. In the past year the existing version of PCModel lapsed off of the eDesktop system and can not be reinstalled, creating both a need and a potential solution simultaneously. The chemistry faculty would like to implement a more advanced computational program which can be integrated into all levels of laboratory and lecture courses throughout the curriculum.

The incorporation of PC Spartan modeling software will open doors to molecular modeling and visualization in General Chemistry 1 through a laboratory experiment already developed here at UWF, and will be accessed and used through Organic Chemistry, Advanced Organic Chemistry, Physical Chemistry and numerous advanced courses. The wide availability of software like PC Spartan will also encourage new and innovative experiment and course design by faculty across all levels of the Chemistry curriculum. Both supplements to existing projects and new “whole-cloth” experiments for every level of experience can be developed with the support of a program like PC Spartan. Finally, having access to 20 licenses will allow for the construction of a Special Topics course in Computational Chemistry to better prepare junior and senior students for graduate coursework as well as for entry into different both industrial and government workforces.

2. Alignment with UWF Strategic Plan

The project is aligned specifically with UWF Priorities 2.1 and 2.3 from the University of West Florida Strategic Plan.

University of West Florida Strategic Priority 2.1 is to respond to the changing need of the region, state and nation by investing strategically to support innovative instruction and high-quality, relevant and distinctive academic and research programs. This project is in alignment with this priority insomuch as the changing nature of jobs in Chemistry requires some level of proficiency with computational and modeling techniques. This program would afford all our majors as well as the numerous disciplines supported by General and Organic Chemistry access to this experience. Having a unified molecular modeling and computational component throughout the Chemistry curriculum would elevate the program and make it unique among peer institutions as well as better preparing our students for careers in a modern chemical workplace.

University of West Florida Strategic Priority 2.3 is to build a vibrant culture of scholarship and research that aligns with UWF's strengths and capacities and supports UWF's

mission, vision and values. The implementation of a computational chemistry component would enhance both the academics of chemistry as well as the numerous undergraduate research projects by affording the wide variety of research chemistry taking place at UWF access to a new tool to enhance research productivity and analysis. This is wholly in line with the mission of the University, which includes enhancing educational achievement. Computational components of General and Organic Chemistry in particular will elevate student learning and help UWF students achieve the learning objectives that will propel them into the workplace, graduate school and professional schools beyond UWF.

3. Description of Benefit Provided

a. Ways in which student access to technology will be enhanced

Through the existing network of computers in Buildings 58 and 58A, students would have the ability to access a modern, sophisticated computational chemistry platform that will be integrated throughout the chemistry curriculum. By purchasing a perpetual license using ITEP funds many years of students in a wide variety of STEM disciplines will gain access to a powerful tool for reinforcing molecular structure, reaction analysis and conformational preferences in addition to a wide variety of other uses as desired by lecture and lab faculty. This impact will persist well beyond the two year time frame of this proposal.

b. How the student experience will be enhanced

Students will gain first hand experience that reinforces concepts taught across the curriculum. Currently the student experience is limited to the visualizations presented in textbooks or online. With access to PC Spartan students will be able to generate models for themselves, manipulate models in three dimensions and study the properties of molecules and behavior of reactions in new and unique ways

c. How assessment will be conducted

All courses and laboratories using computational modeling as a part of the curriculum will be asked to conduct a brief survey on the completion of the project, experiment, or course to assess student perception of learning as facilitated by the computational platform. Assessment will be conducted using Qualtrics (available on my.uwf). Qualtrics assessment will facilitate the simple assessment and reporting of data for large classes such as General Chemistry laboratories in addition to smaller populations such as upper division courses or smaller lab classes. A summary of questions to be asked using the Qualtrics platform is included in Appendix A.

d. Which and how many students will be impacted

The impacted students per existing implementation plans are all students taking General Chemistry 1 Laboratory (~600 students per year), Organic Chemistry 1 Laboratory (~220 students per year) and Organic Chemistry 2 Laboratory (~180 students per year). Depending on instructor incorporation I also foresee impacts in Organic Chemistry 1 Lecture (~250 students per year), Organic Chemistry 2 Lecture (~200 students per year), Organic Chemistry 3 (~40 students per year) and Advanced Laboratory Techniques (~40 students per year). Incorporation by additional faculty will broaden these numbers. There is naturally some double counting of impacts as most students take a lecture and its lab simultaneously, but from a student impact perspective each used of the PC Spartan software will be assessed separately.

e. How students with special needs or disabilities will be helped

The computer labs where the PC Spartan software will be utilized are all ADA compliant. Students with special needs or disabilities have equal access to all these facilities. Additionally, Teaching Assistants will all be trained on use of the software to assist any student with additional needs in the efficient operation of the program to achieve the stated learning objectives.

f. How training of students and faculty in the use of technology would be enhanced

All faculty using the program will have access to training and instructional materials. For laboratory courses taking advantage of the software training will be provided for teaching assistants as well. Students using the software will receive a variety of printed and electronic instructions and guides to facilitate proper use of the software with Teaching Assistants and Faculty available to fill in gaps in understanding and analysis.

4. How Student Success will be Measured

Student success will be determined by the number of students using the software in classes across the curriculum as well as by the outcomes of the Qualtrics assessment of student perception. In particular, questions geared toward determining the extent to which PC Spartan enhanced understanding and retention of topics taught in lecture or laboratory will be used to assess the long term impact of a unified computational platform across the curriculum on student understanding and achievement of Student Learning Outcomes.

5. Resources Needed for the Project and Ongoing Resource Needs

Initial investment of \$12,300 is needed to procure the software. That value accounts for \$8000 to procure the 20 user perpetual license for PC Spartan Student v.7 for student use as well as \$4300 for five individual faculty licenses to develop experiments and courses integrating the use of the software directly. The faculty component is essential for development of experiments and projects for students to undertake as part of course and lab work. Because the licenses are perpetual licenses there is no maintenance or upkeep on the software and thus no ongoing resource needs. The initial costs of the license procurement are the only expense for this project.

6. Project Timeline

- a. Month 1 - Software acquisition, License installation in conjunction with ITS, testing operation of software on computer clusters to ensure ease of access for students.
- b. Month 2 - Faculty and staff training as appropriate for Fall 2016 Courses
- c. Fall 2016 - Incorporation into CHM2045L (General Chemistry 1 Lab) through the Molecular Geometry experiment developed at UWF by Judith Roth (Undergraduate Research student) as well as in Lectures and laboratories per instructor interest. Particular opportunities exist in the Organic Chemistry 1, 2 and 3 (CHM 2210, CHM2211 and CHM3230 respectively) courses as well as Advanced Laboratory Techniques (CHM3740L)
- d. Spring 2017 - Expansion of the software into regular experimental use in Organic Chemistry 1 & 2 laboratories (CHM2210L and CHM2211L) as well as potential expansion into the Physical and Inorganic Chemistry curriculum.
- e. Year 1 - Project review with Qualtrics assessment data and student impact report. Publication of the Molecular Geometry experiment is also expected as the experiment must run with a laboratory course prior to submission for publication
- f. Year 2 - Continued assessment study and course expansion. Final progress report to detail the extent to which the software has been used throughout the curriculum and the impacted student learning outcomes. During the two year project a special topics course related to computational chemistry will also be developed.

7. Sustainability

As the license option being procured is a perpetual license the purchase is sustainable with no further financial or technological inputs needed. At some point in the future (likely 5+ years) it may be advantageous to upgrade to a more current version of the software which could be supported through Laboratory fees or other grant writing activity.

8. Principal Investigator

Dr. Christopher Nicholson, Assistant Professor of Chemistry

Additional Participating Faculty:

Dr. Alan Schrock

Dr. Tanay Kesharwani

Dr. Korry Barnes

Dr. Pamela Tanner

General Chemistry Laboratory Instructors as assigned

Organic Chemistry Laboratory Instructors as assigned

Appendix One:

Sample student assessment instruments

On a scale from 1 to 5 (1 being "Not at all" and 5 being "Very Much") please indicate your answer to each of the following:

1. PC Spartan improved my understanding of molecule shape and behavior
2. PC Spartan enhanced my learning in this course
3. PC Spartan was used in ways that reinforce the textbook and lecture
4. PC Spartan gave me a different perspective on the concepts being discussed
5. I felt prepared to use the PC Spartan software for lecture/lab
6. I feel comfortable discussing PC Spartan and computational chemistry with my peers
7. I will emphasize my experience with computational software in job and professional school applications and interviews

What did you find most helpful about using PC Spartan as a part of this course?

What did you find most interesting about the experiment or project using PC Spartan for this course?

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ITS Review Comments

GENERAL COMMENTS:

None.

COMPLIANCE WITH STANDARDS:

No comments.

INFRASTRUCTURE ISSUES:

No comments.

PRICING/COST ISSUES:

No comments.

OTHER SUPPORT ISSUES:

No comments.

SUGGESTIONS TO PROPOSER:

No comments.

For questions regarding ITS comments, please contact:

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