

UNIVERSITY OF LOUISIANA AT LAFAYETTE

STEP Committee

Technology Fee Application

**Build a regularly used computer classroom to
enhance teaching**

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Knierim and Ryan Simon**

Name of Submitter
(Faculty or Staff Only)

Department of Chemistry

Organization

Title: Build a regularly used computer classroom to enhance teaching

Date: 01/12/2023

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Department/College/Organization: Chemistry/Sciences

ABSTRACT:

The objective of this project is to build a small classroom equipped with ten computers in the Department of Chemistry. There are four medium to large classrooms in the chemistry building (Montgomery Hall Rooms: 103, 106, 227 and 230). These four classrooms can be accommodated up to 70 (Rooms 227 and 230) to 110 (Rooms 103 and 106) students and they are heavily used weekly. The chemistry department offers 300- and 400-level courses and maximal student numbers of some 300- and 400-level courses are between 10 and 20. The chemistry department has a new shared Ph.D. Program in Earth and Energy Science and a new Master Program in Industrial Chemistry and the size of the graduate courses is between 10 and 20 students. The higher-level undergraduate and graduate courses often need specialized computational chemistry software packages that enhance students' understanding of the central role of molecular structures and properties in determining chemical reactions. The student access to specialized computational tools allows the chemistry department to continue to meet American Chemical Society curriculum standards because the Committee on Professional Training of the American Chemical Society lists experience with computational chemistry as one of the recommended topics to be covered in all chemistry lecture and laboratory courses. The chemistry department urgently needs a regularly used computer classroom as part of student learning processes. It is estimated that >100 students from five 300- and 400-level courses and all graduate courses each year will be benefited from this proposed computer classroom. Besides the benefit for teaching, this computer classroom will be used by professional societies to enhance interactions among undergraduate and graduate students. In summary, the improvement of student teaching and the exposure to advanced computational tools will strengthen education components of our science curricula and research productivity.

Build a Regularly Used Computer Classroom to Enhance Teaching

A. Purpose of grant and impact to student body as a whole

The objective of this project is to build a computer lab for expanding access to computational chemistry tools for students through the purchase of ten desktop computers and computer tables and chairs by integrating a site license for the Windows PC versions of Gaussian16 and GaussView6 computational chemistry software programs funded by Louisiana Board of Regents. Over the past decade the role of computational chemistry in understanding a wide variety of chemical systems has expanded greatly. The Committee on Professional Training of the American Chemical Society lists experience with computational chemistry as one of the recommended topics to be covered in a chemistry lecture and laboratory courses.

Some aspects of chemistry can be conceptually difficult. An interactive, highly graphics-based teaching style constitutes the best way to ensure a clear understanding of the presented materials by our students. The proposed computer classroom is expected to have two primary results: an accelerated and more positive learning experience, and improved pass rates as students find it easier to comprehend and apply information presented interactively in our classes. An additional benefit for both students and faculty is a reduction of hand-outs and copies, expensive to generate and easily lost. This grant will enable our instructors to create interactive hands-on lessons, display, 3-D structures, graphs and internet-based material, respond dynamically to inquiries, and increase the participation of our students. More specifically, the increasing availability of software, e.g. Gaussian and GaussView (see below), illustrating complex chemical reactions, molecular structures and molecular diagrams make computer visualization a valuable teaching aid in chemistry courses. Complicated molecular structures in general, organic, inorganic, and biological chemistry can be assembled piece by piece from the computers in the computer classroom.

The Gaussian program has been developed, revised and expanded over a period of several decades and is the most widely used program for computational chemistry, available in versions that run on computers ranging from PCs to supercomputers. The GaussView program serves as an interface for the Gaussian program, making the calculations more accessible to chemists in all areas of chemistry. It provides tools for constructing input files for the Gaussian program and allows visualization of computational results through display of molecular models showing predicted structures. Installing these programs into the computers in the computer classroom will greatly expand access.

Installing an updated windows version of the Gaussian and GaussView programs and expanding access to computational chemistry for students and faculty on local PCs at UL Lafayette will facilitate expanding use of the Louisiana Optical Network Initiative (LONI) supercomputer clusters. With the introduction of computational chemistry coursework through this proposal it is anticipated that more students will move on to become involved in computational research that makes use of LONI resources. The chemistry faculty currently use LONI for computational chemistry research and envisions an expanding role for such work. For research projects that require supercomputer resources, the Windows GaussView program will be used to prepare input files for submitting Gaussian jobs on LONI. Facilitate the use of LONI supercomputer resources through introducing more students and faculty to the use of Gaussian and the ability to use GaussView on Windows computers to prepare input files and view output from calculations performed on LONI.

The UL Lafayette chemistry department has a good record of attracting high-quality local students as well as students from across the state and country. Since access to state of the art supercomputing clusters is a major consideration for top students who plan to study chemistry in college, the opportunity to work with up-to-date computational chemistry software in addition to the instrumentation available in the department will allow the department to continue to be competitive in attracting students who might otherwise seek opportunities outside of Louisiana. The curriculum enhancements provided by this project will enhance student retention by strengthening the ability for students to connect abstract theory with experimental observations. It will also stimulate student interest in pursuing further studies such as engaging in undergraduate research projects by exposing them to a variety of computational chemistry applications in their coursework. By providing increased access to Gaussian16 and GaussView6 along with the other available software, e.g. VMD, AMBER, ChemDraw, SnapGene, in the department, this project will provide opportunities for more students to carry out undergraduate research projects involving computational chemistry and biology. This not only broadens the range of research projects available to students, but also will allow the department to accommodate a larger number of students taking undergraduate research since additional lab space and reagents/chemicals are not needed in order to expand the number of students pursuing computational research.

Besides regular teaching, this computer classroom will be used by students for group studies and for meetings of student professional societies. Interactions among undergraduate and graduate students are essential college experiences. Students can learn from each other.

B. Projected lifetime of enhancement

We will purchase ten desktop computers and computer desks and chairs. The Department Chemistry has the licenses for Gaussian16, GaussView6, ChemDraw, AMBER and SnapGene that will be installed. The Montgomery Hall 139 (MY 139) is a small classroom that can be accommodated up to ~25 students. MY 139 is perfect to be upgraded to a computer classroom. These desktop computers will be added to the routine maintenance schedule of the department.

C. Person(s) responsible for

Implementation: Wu Xu

Installation: Wu Xu

Maintenance: Departmental committee made of up faculty members

Operation: Faculty of Chemistry Department

Training: Chemistry faculty will conduct training for students.

Budget Proposal

1.	Dell Optiplex	\$1,565/PC
	Quantity:	10
	Total:	\$15,565
2.	Computer Tables and chairs	\$5,000
3.	Software	\$ 0.00

No software is required.

4. Supplies		\$0.00
5. Maintenance	Routine maintenance will be covered by department.	\$ 0.00
6. Personnel	No personnel required	\$ 0.00
7. Other	None	\$ 0.00

TOTAL: \$20,565

D. Other relevant information

None

E. Previous STEP projects

Drs. Xu, Gallo and Knierim successfully authored the STEP proposals "Smart Classrooms in Chemistry".