1. Name  **GRANT**  **MARIA EUGENIA**  
   Last  First  Initial

2. Present Assignment  **CHEMISTRY INSTRUCTOR**

3. Number of Years of Full-Time Consecutive Service at Ohlone College  **6 yrs in May 2011**

4. Time period requested for this proposed leave. (Give inclusive dates):  **Fall 2011**

5. Please check which of the following methods you will use to meet the criteria for a sabbatical. Note that "E" is a combination of two or more of the first four.

   [ ] A. Advanced Academic Study: In your statement in Item 7, include a detailed description of the course of study or research project to be undertaken. A letter of acceptance from the institution to be attended or a letter of acceptance from the individual who will direct the study needs to be forwarded to the committee prior to the commencement of the sabbatical.

   [ ] B. Independent Research or Study: In your statement in Item 7, include a detailed resume of the study or project to be undertaken.

   [ ] C. Travel: In your statement in Item 7, include a comprehensive itinerary of your travel plans.

   [ ] D. Employment: In your statement in Item 7, include a complete description of the duties to be performed during the period of employment. Give the inclusive dates of the period of employment. Attach a letter from the employer which confirms the employment and states the salary to be earned.

   ✧ E. A combination of the above activities: In your statement in Item 7, explain carefully how the activities are related and the special results that can be expected. Describe in detail the combination plan in which you are interested.

   [ ] F. Other.

6. On a separate page, write an abstract of this proposal—not to exceed 200 words. This abstract will be presented to the Board of Trustees if this application is recommended for approval.

7. Narrative Description of the Proposed Program—not to exceed five pages.
   Provide comprehensive information about the type of program you selected in part 5. Include detailed information showing how the proposed program will aid or improve the execution of your assigned professional duties and the specific benefits to be accrued to the division/department, district, and students. Explain why a sabbatical leave, rather than other approaches, is required to accomplish the stated purpose. Disclose all information relative to any compensation you will receive during the leave period, other than expense reimbursement, whether from employment, grant, fellowship or any other source which is an integral or related part of the leave program.
To Be Completed by Division Dean before the Application is Submitted:

[ ] I support this application    [ ] I do not support this application

Comments: The General Chem labs need a technology upgrade

Signature of Division Dean  2-1-11

I submit this application with the understanding that I shall be bound by the policies and regulations of the Fremont-Newark Community College District and the Laws of California relating to the granting of Sabbatical Leaves of absence.

Date

FOR COMMITTEE USE ONLY

[ ] Recommended    [ ] Not Recommended

VPI

CHAIR

To those applicants whose proposals are not recommended:

[ ] Due to the intense competition this year, your proposal was not approved. Please consider re-applying in a future year.

[ ] If you wish to resubmit this proposal in a future year, it will require revision in order to show that it meets the following criteria as listed on page one:

[ ] A    [ ] B

[ ] Recommended    [ ] Not Recommended

Comments:__________________________________________________________

Signature of Superintendent/President

[ ] Approved    [ ] Not Approved

Action taken by Governing Board ____________________________________  Date
Abstract:

The activities to take place during the one semester long sabbatical for Fall 2011 are the following:

1. Study via online courses or self study open-source software that is based on modern density-functional-theory for electronic structure calculations and materials modeling at the nanoscale.
2. Use of these methods and tools to create new exercises, dry labs and demos in the chemistry curriculum, updating the existing laboratory protocols.
3. Survey the literature on high temperature superconductors specifically Pr-123 as preparation for a review paper in a peer-reviewed journal.
Background

When I joined the chemistry faculty at Ohlone six years ago, one of the activities I became part of was a departmental effort to modernize the general chemistry curriculum we bring to students both in the lecture hall and laboratory. I have seen many advances since that time...we now use a variety of digital technologies to teach and demonstrate various chemical approaches and techniques. Last summer I attended the 21st Biennial Conference on Chemistry Education in Denton Texas and visited there the Department of Chemistry at the University of North Texas. From what I saw and learned, I would argue Ohlone is now on the vanguard of undergraduate chemical education.

At the time I arrived at Ohlone, we were still teaching from the laboratory manual put together by Professor Emeritus James Klent. Then, in 2007, the department received additional funding from the College Council which was used to purchase laptop computers and digitally-controlled experimental probes to aid in data acquisition and processing. For example, we acquired automated pH detectors, temperature, conductivity and colorimetric probes and associated software support. Later we also obtained gas pressure sensors and a spectrophotometer.

Since obtaining these new resources, we modified our present laboratory curricula accordingly, and added new experiments as well. The latter went quickly and well, but the former presented more of a challenge. Professor Klent had graciously made the laboratory protocols to the students free of charge, they were subsequently posted on webCt for them to download and print.

However, the laboratory session documentation for both Chem 101A and B lacks uniformity. There are many protocols that must be changed, not only due to the use of new textbooks, but also due to the data acquisition tools available on our new equipment. For example, a typical protocol followed by Prof. Klent required the students to manually prepare a table in which to enter various experimental observations, e.g., volume readings and associated pH values. Now it is possible to carry out these operations, and others, employing a GUI (graphical user interface), but a new student protocol is needed to accommodate using these modern tools and the instructions in the proper software language have to be written.

As an important aside, with these new tools, being more sensitive in nature, we can use smaller amounts of chemicals and hence generating less waste. Ohlone's chemistry laboratories are transitioning from doing toxic and hazardous chemistries towards sustainable green chemistry. This way we will not only use fewer chemicals that are toxic to humans but will have lower costs, use less energy and other resources in general.
I have been gradually modifying the laboratory protocols, but am time limited by general teaching requirements during each school semester and much more work needs to be done.

We are advancing the chemistry curricula to include modern quantum chemistry techniques. I consider this to be a critical area for today's chemistry students to become aware of. I believe in the future most forefront chemistry synthesis research will begin "in the computer" before moving to the traditional "wet" lab. We have obtained two software products from Wavefunction, Inc., Spartan and Odyssey, the former a powerful commercial product for chemical industry and pharmaceutical research, and the latter a "teaching" tool used at different levels throughout high school, college and university chemistry curricula. These programs combine advanced molecular graphics visualization. Spartan also allows the use of elementary "Hartee-Fock" techniques to emulate and visualize synthesis of simple molecules through minimizing their total ground state (equilibrium) energies as a function of atomic arrangement (e.g., computing the H-O-H bond angle in water, responsible for its polarization properties and the basis of life on earth). Right now, we have only two lab sessions in which the students use Spartan...there could be considerably more...to explore issues of polarity and infrared spectra (e.g., the "greenhouse gas" effect). The Wavefunction products are proprietary and expensive, licensed to only one machine at a time, we currently have 15 of them for a class of 30 students. There are now available open-source software packages more powerful, free and maintained by a worldwide user community.

I am now eligible to apply for sabbatical leave. I would like to do so and I am proposing a tentative program, which would not require relocation from the Bay Area.

Activities during the sabbatical leave:

1) I will review, edit and modify the current laboratory protocols to accommodate the new instrumental facilities, and write, when needed, the additional software that is necessary. These protocols will be standardized across laboratories and, of course, made available to instructors and lab technicians alike, with equipment photographs and other visuals, on a CD and free of charge to the students via Blackboard or WebCT.

2) I would pursue either by self-study, or via on-line courses, use of modern density-functional-theory tools and methods (DFT won the 1998 Nobel Prize in Chemistry) as open-source adjuncts to Spartan and Odyssey (unlike the latter, DFT techniques are equally applicable to crystalline solids such as semiconductors, superconductors, graphene and nanotubes, as well as molecules). The two major sources of open-source DFT packages are Quantum-Espresso and ABINIT. The former is used as the basis of undergraduate courses in materials chemistry at a number of universities throughout the world not necessarily carrying a pre-requisite in quantum mechanics 1. I will explore on-line courses offered at such institutions. The objective would be to use these leading-edge...and freely available...resources to provide examples and exercises for Ohlone students taking physics and chemistry courses to explore what is rapidly becoming a major tool for research in materials science.
3) 2011 is the 100th anniversary of the discovery of superconductivity, and the 25th of the discovery of "high temperature" superconductivity in IBM in 1986. In 1987, the IBM Almaden Research Center in San Jose played a major role in extending the transition temperature of these compounds, especially a perovskite system known as "yttrium-123." It was found that all members of the rare-earth element family when substituted for yttrium in the "123" lattice resulted in superconductors as well...except one...praseodymium. Why not Pr remains a mystery and one of the major issues in superconductivity to this day. In 1989, as a visiting scientist at IBM Almaden on sabbatical from UNAM, I conducted research on this compound and this question. My paper\(^2\) became one of the most cited in the field of high temperature superconductivity. As a sabbatical project, I would like to survey the extant literature on Pr-123 as preparation for a review paper in a peer-reviewed journal such as Chemical Reviews. I would use this experience to advance my mentoring skills for Ohlone students considering continuing on to graduate study in chemistry in the UC system or elsewhere. In other words, to respond to questions like "What's it like to become a chemistry researcher in an exciting forefront field?" The principal resource I would need is on-line access to the UC library subscriptions, which I would explore obtaining, perhaps establishing a precedent for Community College faculty in general.

1. e.g. Atomistic Computer Modeling of Materials, Prof. Nicola Marzari, MIT Open Courseware, via iTunes U.
2. Quantum Espresso tutorial; http://www.fisica.uniud.it/~giannozz/QE-Tutorial/