UNIVERSITY OF THE PACIFIC
GRADUATE COURSE APPROVAL FORM

Please fill in all information. After all required signatures are obtained on page two, send to Research and Graduate Studies, Knoles Hall, 2nd Floor. Research and Graduate Studies will then forward to the Academic Affairs Committee, Office of the Provost, Anderson Hall, 2nd Floor.

**Date:** August 8, 2006
**Contact Person:** Elfi Kraka
**Department:** Chemistry
**Phone:** 946-2967

<table>
<thead>
<tr>
<th>Please mark one:</th>
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<tbody>
<tr>
<td>ADDITION ✔</td>
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<tr>
<td>REVISION</td>
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<tr>
<td>DELETION</td>
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<table>
<thead>
<tr>
<th>School or College: COP</th>
<th>Department: Chemistry</th>
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<tbody>
<tr>
<td>Course Number: PCSP 243</td>
<td>Title: Applied Computational Chemistry</td>
</tr>
<tr>
<td>Minimum Number of Students: 4</td>
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<tr>
<td>Prerequisites: Graduate standing or permission of instructor</td>
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If replacing a course, old course title and number:

Catalog Description: Besides the normal laboratory experiments traditionally expected, modern chemists/biochemists, whether in the chemical/pharmaceutical industry or academia, perform “experiments” on the computer by calculating the outcome of chemical and biochemical reactions. This *in silico* chemistry has become an integral part of the education in chemistry and the present course will provide an introduction into this new field by addressing a general audience of chemists/biochemists and students from neighboring fields. *Prerequisite: Graduate standing or permission of instructor.*

Please attach a syllabus.

What are the reasons for the new course (e.g., student needs, major, etc.), program changes or deletion of the program?

Important new course for the nanotechnology track.

If approved, when will this be implemented?

Spring, 2007
What is the anticipated impact on resources (Faculty, funds, library materials, etc.)?
None

Describe any special facilities, furnishings, or technology needs. List software needs, if any.
Computers and software provided by the department of chemistry.

APPROVAL PROCESS

1. Action by department requesting addition/change:
   Approved by: [Signature] Date: 10/20/06

2. Action by the Curriculum and/or Graduate Studies Committee of the School/College:
   Approved by: [Signature] Date: 10/20/06

3. Action by the Dean of the School/College:
   Approved by: [Signature] Date: 10/20/06

4. Action by the Dean of the Library:
   Approved by: [Signature] Date: 10/20/06

5. Action by the Director of Educational Technology Services (if computer lab, software needed):
   Approved by: N/A Date: 

6. Action by the Registrar:
   Approved by: [Signature] Date: 11/13/06

7. Action by the Graduate Studies Committee (as appropriate):
   Approved by: [Signature] Date: 11/16/06

8. Action by the Academic Affairs Committee:
   Approved by: Date: 

After approval by the Academic Affairs Committee, information regarding new, revised, or deleted courses is sent to the Registrar for listing in or modifying the catalog.

Form revised: 9/4/03
1.) JUSTIFICATION FOR THE COURSE: Teaching in the year 2006 requires besides the basic didactic virtues also flexibility and creativity. New fields and disciplines have to be integrated in the syllabus without jeopardizing well-established standards. However, the student must be prepared for the rapid changes taking place in industry and the working world in general. This course will prepare graduate students in organic, inorganic, physical, biochemistry, medicinal chemistry, and pharmaceutical sciences for situations in the working world that requires in silico chemistry to improve the budget of a chemical or pharmaceutical company (a chemical experiment may take two months, an in silico experiment just two hours provided the company co-worker has obtained the appropriate education in applied computational chemistry). Performing chemical experiments on the computer is an important part of a modern graduate education, which is missing so far in the PCSP curriculum.

2.) STAFFING NEEDS: Graduate faculty

3.) ESTIMATED CLASS ENROLLMENT: minimum of 4 students

4.) ANTICIPATED IMPACT ON CLASSROOM FACILITIES: A lecture/discussion room and a computer lab will be needed for this course.

5.) ANTICIPATED IMPACT ON ELECTRONIC TECHNOLOGY: Current ET facilities are adequate.
COURSE SYLLABUS

Pharmaceutical and Chemical Sciences Graduate Program

Course Date: August 8, 2006

<table>
<thead>
<tr>
<th>Course Number</th>
<th>Course Title</th>
<th>PCSP 243</th>
<th>Applied Computational Chemistry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Department</td>
<td>Instructor(s)</td>
<td>Chemistry</td>
<td>Elfi Kraka</td>
</tr>
<tr>
<td>Number of Weeks</td>
<td>Maximum Enrollment</td>
<td>13</td>
<td>20</td>
</tr>
<tr>
<td>Lecture Hours per Week</td>
<td>Laboratory Hours per Week</td>
<td>4</td>
<td>4</td>
</tr>
<tr>
<td>Discussion Hours per Week</td>
<td>Number of Labs per Semester</td>
<td>0</td>
<td>30</td>
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<tr>
<td>Unit Value</td>
<td>Experiential Hours per Week</td>
<td>4</td>
<td>0</td>
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Course Description: Starting from the description of atomic and molecular electronic structure, then discussing the elementary processes of bond breaking and forming, the course leads to the calculation of typical chemical reactions in a hands-on fashion. Major quantum chemical packages will be used for this purpose.

Prerequisites:
Graduate standing or permission of instructor

Teaching Methodology:
Lectures and computer labs

Evaluation Methodology:
The University Honor Code is an essential element in academic integrity. It is a violation of the Honor Code to give or receive information from another student during an examination, to use unauthorized sources during an examination, or to submit all or part of someone else's work or ideas as one's own. If a student violates the Honor Code, the faculty member may refer the matter to the Office of Student and Professional Affairs. If found guilty, the student may be penalized with failure of the assignment or failure of the course. The student may also be reprimanded or suspended from the University. A complete statement of the Honor Code may be found in the Student Handbook, "TIGER LORE".

Attendance is expected at all class sessions.

Class assignments may be retained by the instructor to assess how the learning objectives of the course are met.

The instructor may be contacted during office hours or _x_ by email, _x_ phone, or _x_ via Blackboard.com.

Weighting of Assignments:

<table>
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<tr>
<th>Assignment</th>
<th>Weight</th>
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<tbody>
<tr>
<td>Final Exam</td>
<td>50%</td>
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<tr>
<td>Quizzes</td>
<td>30%</td>
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<tr>
<td>Lab reports</td>
<td>20%</td>
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Assignment of Grades:

<table>
<thead>
<tr>
<th>Grade</th>
<th>Percentage</th>
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<tr>
<td>A</td>
<td>90%</td>
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<tr>
<td>B</td>
<td>80%</td>
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<tr>
<td>C</td>
<td>70%</td>
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<td>D</td>
<td>60%</td>
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<td>F</td>
<td>&lt;60%</td>
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<tr>
<td>GOALS</td>
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At the end of the course the student

- will be able to describe the concepts of the laws of quantum mechanics necessary for the description of atoms and molecules and their chemical reaction;
- will be able to choose the appropriate method (in terms of applicability, accuracy, and economy) for the calculation of a given chemical problem;
- will be able to describe, perform, and interpret the results of the calculations and bring them to a publication ready form.
OBJECTIVES

The course will discuss the basic principles of quantum mechanics which are necessary to understand the properties of atoms and molecules and their chemical reaction. A variety of different methods for the calculation of molecular properties will be systematically discussed, ranging from very accurate methods for small molecules to less accurate methods for large molecules. The material will be presented in a form that a chemist, biochemist, or medicinal chemist can follow without getting lost in mathematical derivations and difficult equations.

The methods discussed will be applied in the computer labs to solve typical chemical problems, which are taken from the actual research in the theoretical chemistry group. In this way the student gets a realistic training in how to use computational tools in his/her studies or later career in academia or private industry.
COURSE SYLLABUS
Pharmaceutical and Chemical Sciences Graduate Program

COURSE OUTLINE
Didactic Sequence and Time Allotment
(Attach Additional Page(s) if needed)

Instructor: Dr. Elfi Kraka

Contact Information:
Office Room: CR 174 (Classroom Building)
Office Hours: MF 12:30-1:30 p.m. and by appointment
Office Phone: 209-946-2967
Electronic Mail: ekraka@pacific.edu

Texts:
b) Handouts and notes for the computer labs

Schedule
In 14 chapters, the course leads from early quantum theory to modern ab initio calculations (13 weeks, 26 lectures, 100 minutes each)

1. Early Quantum Theory: historical overview; influence of physics on Theoretical Chemistry; blackbody radiation; photoelectric effect; Bohr and the H atom; de Broglie wavelength; Heisenberg uncertainty principle.
2. The wave equation: differential equations, separation of variables.
3. The Schrödinger equation and simple applications such as the particle in the box.
4. Basic Quantum Mechanics: state of a system; operators and observables; postulates and general principles of quantum mechanics.
5. The Harmonic Oscillator: diatomic molecules; solution of the harmonic oscillator problem; quantum mechanical tunneling.
6. From one to three dimensions: particle in the 3-dimensional box; the rigid rotator; the hydrogen atom; quantum numbers; orbitals.
7. Approximated methods: independent particle approximation; variational method; perturbation theory.
8. Calculation of atoms: application of variational method and perturbation theory to the He atom; Hartree-Fock calculation of the He atom; electron spin and Pauli principle; antisymmetric wave functions and Slater determinants; singlet and triplet wave functions; atomic term symbols.
9. Calculation of molecules: Valence bond theory of H2; chemical bonding; Molecular Orbital Theory; theory of H2+ and H2; improvement of valence bond theory; generalized valence bond; configuration interaction with single and double excitations.
11. Ab initio theory: basis sets; restricted and unrestricted Hartree-Fock; electron correlation; many body perturbation theory; couple cluster theory; multi-configuration self-consistent field theory.
14. Mixed methods like the combination of quantum chemical methods and molecular mechanics (QM/MM) for the description of biochemical problems, for example, the interaction of a drug and a receptor.
Ten mandatory computer labs complement the lectures. In these labs the students learn how to solve chemical problems by means of ab-initio theory and Density Functional Theory calculations. Examples are taken from current research within theoretical chemistry (e.g. problems from atmospheric chemistry, anti-cancer chemistry, etc.) Students will be trained in how to calculate molecular properties as energy, geometry, vibrational frequencies, NMR chemical shifts, dipole moments. Advanced topics are modifications and design of basis sets, calculation of reaction rates by means of variational transition state theory, reaction path following, and the description of a biochemical problem with QM/MM. The emphasis will be on using the best possible method and basis set (according to accuracy and economy) for a given problem. How to derive chemical important information from the numbers produced, how to bring the results to a form ready for publication will be discussed.