Chemistry 501
Computational Physical Chemistry
MW 1500-1700
Fall 2015

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Introduction: This course presents an introduction to computational chemistry methods as applied to physical chemistry. Topics to be introduced and discussed include: molecular modeling with classical force fields, semi-empirical and *ab initio* quantum mechanical methods, Monte Carlo and molecular dynamical methods, and quantitative structure activity analysis (QSAR). The content of this course will include some background theory and applications of the various modeling techniques and a number of hands-on activities using available software.

Course Description: Introduces students to computational methods as applied to some of the major theoretical ideas of Physical Chemistry. The concepts to be covered will include examples from: Classical Chemical Thermodynamics, Statistical Thermodynamics, Chemical Kinetics, Quantum Chemistry, and/or Molecular Modeling. The course is designed to build on previous knowledge of Physical Chemistry gained at the undergraduate level.

Prerequisites: The prerequisites for this course are successful completion of one full year of Physical Chemistry (CHEM 401 and CHEM 402).

Text: There is no specific text for this course. Readings from the literature will be used to introduce certain concepts. Students will be required to consult the primary literature for examples of various research applications of the various computational methods that have been studied. In addition, the instructor will provide supplemental reading material as required.

Topics

1. $\Delta H°$ as a Function of Temperature
2. Determination of $\Delta H°$ Using the van't Hoff & Claussius-Clapeyron Equations
3. A Statistical View of S
4. Calculation of $\Delta G°$ and K as Functions of Temperature
5. Chemical Kinetics Using Differential Equations
6. Rate Processes Using Stochastic Simulations
7. Atomic Structure and Spectra
8. A Molecular Orbital Description of Bonding
9. Potential Energy Surfaces of Molecules
10. Spectroscopic Properties of Molecules
11. Potential Energy Surfaces for Non-covalent Interactions
12. Classical Models for Potential Energy Surfaces
13. A Theoretical Description of Chemical Reactions
14. Spectroscopic Properties of Molecules from Quantum Mechanics
15. Quantitative Structure Property Relatiionships (QSPR)

Student Learning Outcomes: During this course students will:

1. Apply computational simulation methods to predict the behavior of chemical systems.
2. Investigate how chemical and physical parameters affect experimentally observable quantities as given by the fundamental equations of physical chemistry.
3. Examine statistical relationships between various chemical and physical properties of molecules.

4. Apply quantum mechanical methods in order to predict reaction energies, molecular structure, and spectroscopic properties.

Grading: The course grade will be determined by the student's performance on in-class exercises, short written reports, mini-projects, and the final exam.

Item	**Points**
In-class Lab Reports (13 x 20 pts)	260
Short Literature Reports (4 x 100 pts.)	400
Mini-Projects (2 x 120 pts.)	240
Final Exam	100
	1000

A- ≥ 900; B- ≥ 800; C- ≥ 700; D- ≥ 600 (absolute point scale)

The final exam is scheduled for: XX from YY-ZZ.

In-class Lab Reports

These reports will be due at the end of class and will be a summary of the computational work you have done in that day's class. Needless to say, you must attend class in order to complete these reports.

Short Literature Reports

These reports are based on a publication from the primary literature that you have chosen to read. After reading the paper you are required to write a two page (word-processed, 12-pt font, 1 inch margins) summary of the paper. The summary should include sections on: (i) the purpose of the work, (ii) the computational methodology used, (iii) the relevant data obtained, (iv) the conclusion, and (v) a critique of the computational methodology used to solve the problem. Appropriate publications will be chosen in consultation with the instructor, although it is the responsibility of the student to search the literature for the publications to be considered.

Mini-Projects

These will be short assignments in which you will be asked to solve a chemical problem using computational methods that have been presented in class. A short abstract (300 words or less) as is usually written for a formal publication is required. This abstract should concisely describe the purpose, methods, major results, and conclusion of your research. In addition, you will need to turn in publication quality tables concisely summarizing all of your calculations.

CSUSM Writing Requirement

The University writing requirement will be satisfied through the written lab reports for the in-class computational exercises, the literature reports, and the reports for the mini-projects.

Office Hours: My official office hours for the semester will be: XXX. I also encourage you make an appointment to see me at other times if you need help.