

## Course syllabus for Chemistry 126 / 226 Computational Chemistry

Class meets:	Tue, Thu	8:00 – 8:50 AM	<b>Buchn 1934</b>
Comp. lab:	usually every other Tue	8:00 – 8:50 AM	<b>Chem 1153</b>

**Instructor:** Dr. *Kalju Kahn*, Office: PSB-N 2623,  
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Office Hours: Tue and Thu (11:00-12:00 PM) or by appointment  
Course website: <http://www.chem.ucsb.edu/~kalju/chem126>

### **Lecture Textbooks:**

Required: Frank Jensen  
Introduction to Computational Chemistry, 2<sup>nd</sup> edition (Wiley)

or

Christopher Cramer,  
Essentials of Computational Chemistry, 2<sup>nd</sup> edition (Wiley)

Recommended: Andrew Leach, Molecular Modelling: Principles and Applications, 2nd Edition (Prentice Hall). This book is usually used in Chem 145 (Computational Biochemistry)

### **The Course:**

The course focuses on learning the principles of [computational chemistry](#) and computer-based molecular design. Both molecular mechanical and quantum mechanical models are covered. Students will learn a variety of commonly used techniques, such as geometry optimization, location of transition states, conformational analysis, and prediction of molecular and spectroscopic properties. Students will learn basics of implementing key algorithms, such as Newton-Rhapson minimization, and normal mode analysis of vibrational motions. Students also will become familiar with different software packages, including [MOLDEN](#) for general model building, [Gaussian](#), [Firefly](#), and [NWChem](#) for quantum chemical calculations, and [BOSS](#) for liquid simulations. Students who complete the course are expected to be able to ask questions that can be solved with modern computational approaches and choose right computational tools to assist in their current or future research.

### **Expectations of Students:**

- Attendance and taking good lecture notes is expected. Submitting completed assignments in time is required.
- The course involves significant hands-on experience with computers. Students should learn how to independently use Linux-based operating systems and computational chemistry software. Good knowledge of elementary calculus and ability to learn simple computer programming are expected.
- The textbook provides most of the necessary background material. Furthermore, students are expected to read and critically analyze modern computational chemistry-related research literature. Required literature will be available on the course website.
- Honesty and academic integrity must be always preserved. While discussing your ideas with others is encouraged outside the classroom, you must answer the assignment questions individually. No supplemental material should be used during an exam.
- Your grade in the course is based on points you collect from the weekly assignments (10 points each), a mid-term (40 points), and a final and/or an independent research project (50 points). Grading will be based on the curve but you have to meet a certain level to get a grade higher than F.

- Students can choose to turn in an independent research project instead of taking the final exam. The quality of the work in the research project shall meet the standards of publication in mainstream computational or physical chemistry journal. The research project shall not be an integral part of a research project that is concurrently being pursued in the lab that the student is working in.
- The course requires that you have a solid understanding of basic biology and organic chemistry; good background in biochemistry and physical chemistry will be very helpful.
- No student shall give, sell, or otherwise distribute to others or publish any electronically available course materials or recordings made during any course presentation without the written consent of the instructor.

### **Coursework:**

- You are expected to electronically submit six weekly assignments that will be graded. The assignments will be posted to the course website and you will typically have seven to nine days to complete each assignment. I will usually post the assignments on Monday. The class will meet on some Tuesdays in the computer lab where you will learn some of the steps necessary to complete the assignment. I am able to help you with your assignments if you are stuck. The assignments are due on midnight on Thursday of the next week.
- I recognize that course like “Computational Chemistry” may seem challenging to students who are not used to working with computers. To allow students with different computer and math skills be successful in the course, I have divided the problems into three levels as explained below.
  1. The first level problems are straightforward. They can be readily solved based on examples, lecture materials and the textbook. Computational problems at this level would not present any unusual challenges to students. This level is recommended to students who feel that their math and computer skills are weak but who still want to learn the basics of computational chemistry. The undergraduate students who take a path of answering only first level problems are unlikely to get a grade above B because the maximum number of points for each first level weekly assignment is 7 / 10. Graduate students (Chem 226) should not turn level one assignment in for grading.
  2. The second level problems are more difficult. To solve these, most students would spend some time analyzing the problem and carefully thinking what has been taught in the course. However, these problems are solvable within the scope of the material covered. Computational problems at this level may be more challenging: it is possible that your first calculations do not converge to desired result and you may need to do significant post-calculation analysis. The undergraduate students who take a path of solving second level questions could get A+ because each assignment is maximally 10 / 10. Graduate students may turn these assignments in for a maximum grade of 8 / 10
  3. The third level problems are challenging. Finding a solution to these involves considerable independent thinking and/or work with the scientific literature. The calculations at this level are more demanding and students wishing to take this path may want to install some computational chemistry software on their personal computers. Answers to level three questions also typically require some literature research in order to compare your results with experimental data, published calculations with other methods, and to rationalize the results. Undergraduates who successfully solve level three problems are likely to receive A+ because these are graded on 12 / 10 basis. Graduate students are expected to solve most level three problems and receive maximally 10 / 10 for each.

Each undergraduate can of solve and submit answers to questions at different levels. If you submit multiple level answers, the grading works as follows: I will first grade your highest level assignment, and if you have less than the maximum there, I will grade the lower level assignment and add the

points based on the formula 
$$P_{added} = P_{low} * \frac{P_{high}^{max} - P_{high}}{10}$$

For example, if you got 5 / 10 on the second level and 7 / 10 (maximum possible) on the first level question, your final score will be 
$$P_{final} = 5 + 7 * \frac{10 - 5}{10} = 8.5$$

What if you decided to try the third level and got 4 there along with a maximum 7 / 10 on the first level? Now your score will be: 
$$P_{final} = 4 + 7 * \frac{12 - 4}{10} = 9.6$$

Thus, it pays to do the lower level problems if you think that your higher level is not very strong. On the other hand, if you are confident that your high level answer is nearly perfect, you may ignore the lower level.

### ***Study tips:***

- **Start your homework or research project early. It is common that calculations take several hours, if not days. It is unlikely that you can complete your assignment in less than a day because your calculation may wait in the queue for many hours.**
- Check your calculations frequently to make sure that things go as you expect. We do not grade on the computer time you spend but on the results you get. Submitting a wrong answer with explanation that you accidentally had +1 for the charge instead of -1 will do no good.
- Come to the lab prepared. Think what you want to accomplish **ahead** of time; look up the chemical structures of molecules you plan to construct, work out any necessary math. We have over twenty students, about one hour, and only one instructor!
- Come to the lecture prepared. Read the relevant textbook material and required reading **before** the class meets. I like to interact with students during our meetings and you enjoy the lectures more if you can think along.
- Review (or rewrite) your class notes the same day and supplement them with material from the textbook and other resources (optional reading, Internet). Ask for help if something remains unclear.
- This course is not about memorization of names, reactions, or facts. It is about understanding the process, its principles and methods. You should demonstrate good understanding of the material when answering assignment questions and the exam problems. Your creativity and originality are highly important for getting a high score in the project if you choose to carry out one.

*Good luck! — Kalju*

**Chem126/226****Schedule for the Fall 2011**

Sept 22		Overview of the course. Promises of computational chemistry.	
Sept 27	Lab 1	Minimization algorithms	
Sept 29		Molecular mechanics: Molecular mechanics of bond vibrations. Minimization methods	
Oct 4		Forces in polyatomic molecules; parameterization and testing of force fields	
Oct 6		Monte Carlo method: Principle and applications	<b>First assignment due</b>
Oct 11	Lab 2a	Force fields and conformational analysis	
Oct 13	Lab 2b	Monte Carlo simulation of solutions and liquids	
Oct 18		Quantum mechanics. Semi-empirical MO theory	
Oct 20		Hartree–Fock Theory: Principles and applications	<b>Second assignment due</b>
Oct 25	Lab3	Semi-empirical methods	
Oct 27		Ab Initio MO Theory: Basis Sets	
Nov 1		Treatment of electron correlation: wave function methods	
Nov 3		Treatment of electron correlation: density functional theory	<b>Third assignment due</b>
Nov 8	Lab 4	Computer Lab: Hartree-Fock theory; molecular orbitals	
Nov 10		Vibrational spectroscopy and gas phase thermodynamics	
Nov 15		Reaction paths and transition states in gas the phase reactions	
Nov 17		<b>Mid-Term examination</b>	
Nov 22	Lab 5	Computer Lab: molecular vibrations and transition states	<b>Fourth assignment due</b>
Nov 24		<b>Thanksgiving Holiday</b>	
Nov 29		Description of electronically excited states	
Dec 1		Description of solvent effects	<b>Fifth assignment due</b>
Dec 6	Lab 6	Prediction of optical spectra and solvent effects	
Dec 8		Open	
Dec 8			<b>Course projects due</b>
<b>Dec 12</b>			<b>Sixth assignment due</b>
<b>TBA</b>		<b>Final Exam</b>	

**Assignments:**

1. Minimization algorithms
2. Monte Carlo conformational analysis and simulation of liquids
3. Application of semi-empirical methods to chemical reactions
4. Description of chemical reactivity using MO theory
5. Vibrational analysis and location of transition states
6. Optical spectra and solvent effects