

Chemistry 302: Introduction to Computational Chemistry

Spring 2010

Instructor: Prof. Kevin Range

Office: Ulmer 417

Email: krange@lhup.edu

Phone: 570-484-2959

Required materials: *Essentials of Computational Chemistry*, 2nd ed., Christopher J. Cramer

Lecture: MW - 9:05AM–9:55AM Ulmer 211 (we may meet in 311 a few times)

Office hours: M - 2:00PM–3:00PM, T - 9:30AM–10:30AM, W - 1:30PM–3:30PM, R - 1:30PM–3:30PM, and *by appointment*

Course website: <http://www.lhup.edu/krange/courses/chem302/>

Description: This course serves as an introduction to the field of computational chemistry. Topics covered will include, but are not limited to, molecular mechanics, molecular orbital theory and density functional theory. Students will learn how to perform various computational chemistry calculations and the application of their results. Critical evaluation of computational chemistry results appearing in the scientific literature will also be discussed.

Exams: There will be four exams. The first will cover chapters 1 and 4, the second will cover chapters 6, 9, and 10, the third will cover chapters 7, 8, and 5, and the final exam will be a comprehensive exam for this course.

The first three exams are tentatively scheduled to be on 2010-02-03, 2010-03-03, and 2010-04-07.

The final exam is scheduled for 10AM–11:50AM, 2010-05-07.

Problem sets: There will be a number of problem sets assigned throughout the semester which will require you to perform calculations and report your results.

Reports: There will be several written reports assigned in which you will critique and/or analyze computational chemistry literature.

Attendance: Attending lecture is strongly encouraged. Absence from lecture carries no formal penalty but excessive absences will affect your grade.

If you do not complete a graded assignment due to an unexcused absence you will receive a grade of zero for that assignment and will not be afforded an opportunity to make up the assignment in question.

Absences will only be excused in advance.

If you are unclear in any way about the above attendance policy, please seek clarification as soon as possible. You will be held to this standard whether you understand it or not.

Student responsibilities: You are expected to complete all assignments on time, with academic integrity, and in the manner instructed. Failure to meet these responsibilities will have a detrimental effect on your grade. Specifically, assignments that are late and/or the product of unethical conduct will receive a grade of zero.

Computer malfunction is generally not an excuse for missing assignments. Proper backup practices and use of the technology services available at Lock Haven and on the Internet should allow you to access a relatively recent copy of any data you may need from nearly any computer at anytime.

Grades: Your final percentage grade will be the weighted average of all of your coursework:

Problem sets	Reports	Exams*	Final
25%	25%	30%	20%

* excluding the final exam

Your final letter grade will be computed from your final percentage grade using the fairly standard set of brackets below. The instructor *may* adjust the brackets to give a more meaningful distribution of letter grades. Such adjustments will *never* result in a lower letter grade than that obtained from the brackets below.

**Percentage to letter
grade conversion table**

A	93–100	C+	77–79
A-	90–92	C	73–76
B+	87–89	C-	70–72
B	83–86	D+	67–69
B-	80–82	D	60–66
	E <59		

Academic integrity: Copying of another person’s work, obtaining copies of tests prior to their administration, using unauthorized materials during tests, sharing or stealing information during and exam, and alteration of a graded exam and then requesting a re-grade, plagiarism in any form, and any other violation of academic integrity standards are all forbidden. Violations will result in a grade of zero being assigned for the work in question and may be reported to the proper authorities. For further discussion of academic integrity see the *Student Handbook* http://www.lhup.edu/stulife/student_handbook/index.htm

If you have any questions about academic integrity, plagiarism, or anything else *please* come and see me. I hate having to fail students for violating academic integrity standards and then having them plead ignorance. *Ignorantia juris non excusat.*

Reasonable accommodations for students with disabilities: Students with disabilities are encouraged to discuss requests for reasonable accommodations with the professor at the beginning of the semester. In order for accommodations to be provided, your disability must be verified by Disability Services for Students.