

Syllabus

CHM6440/7440 - Computational Chemistry

Winter 2016

Instructors: H. Bernhard Schlegel 375 Chemistry
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Lectures: Tue, Thu 11:45 AM – 1:10 PM
Rm 025 Chemistry (Computer Lab)

The course will consist of lectures and hands-on computational labs. There will be one midterm (worth 20%), 5 quizzes (15%), 5 computational assignments (30%), and a major computational project (35%).

Prof. Schlegel will teach the first half of the course and Prof. Cisneros will teach the second half.

Learning outcomes: At the completion of the course the students will understand the fundamentals of Quantum and Classical simulation methods and be able to perform calculations on small molecules and biomolecules with the Gaussian09 and AMBER14 software packages. Calculation of molecular properties including vibrational spectroscopy, optimization, thermochemistry, SCF convergence, classical molecular dynamics, Monte Carlo, free energy perturbation methods and hybrid QM/MM methods. In addition, the students will become familiar with high performance computing (HPC) environments. The emphasis will be on the fundamental Quantum and Classical methods behind the simulation procedures and simulation methods.

Suggested Readings:

-**“Exploring Chemistry with Electronic Structure Methods: A Guide to Using Gaussian”**, J. B. Foresman and A. Frisch, 2nd Ed., Gaussian Inc.

-**“Molecular Modelling; Principles and Applications”**, A.R. Leach, 2nd Ed., Prentice Hall.

-**“Essentials of Computational Chemistry”**, C.J. Cramer, 2nd Ed., John Wiley and Sons.

-**“Introduction to Computational Chemistry”**, F. Jensen, 2nd Ed., John Wiley and Sons.

STUDENT DISABILITY SERVICES: If you have a documented disability that requires accommodations, you will need to register with Student Disability Services for coordination of your academic accommodations. The Student Disability Services (SDS) office is located at 1600 David Adamany Undergraduate Library in the Student Academic Success Services department. The SDS telephone number is 313-577-1851 or 313-577-3365 (TDD only). Once you have your accommodations in place, We will be glad to meet with you privately during office hours to discuss your special needs. Student Disability Services' mission is to assist the university in creating an accessible community where students with disabilities have an equal opportunity to fully participate in their educational experience at Wayne State University.

Tentative Schedule:

Week 1, Jan. 12, 14.

Intro to High Performance Computing (HPC) on the Wayne State Grid.
Population analysis and molecular properties, geometry optimization (Jensen Chs. 9-10)

Week 2, Jan. 19, 21.

Vibrational frequencies, transition states, reaction paths (Cramer Ch. 10, Jensen Chs. 12-13)

Week 3, Jan. 26, 28.

Electron correlation, Density Functional Theory (Cramer Chs. 7-8, Jensen Chs. 4,6)

Week 4, Jan 2, 4.

Model chemistries, thermochemistry (Cramer Ch. 10)

Week 5, Feb. 9, 11.

Molecular Orbital Theory (Cramer Chs. 4-5, Jensen Ch. 3, Leach Ch. 2)

Week 6, Feb. 16, 18.

SCF convergence and stability, excited states (Cramer Ch. 13)

Week 7, Feb. 23, 25.

Assorted special topics in electronic structure theory

Week 8, Mar. 1, 3.

Molecular Mechanics; Empirical Force Fields (Leach Ch. 4, Cramer Ch. 2, Jensen Ch. 2)

Proposals for term projects due

Week 9, Mar. 8, 10.

Classical Simulation Methods (Leach Ch. 6, Cramer Ch. 3, Jensen Ch. 14)

Week 10, Mar. 15, 17.

Molecular Dynamics (Leach Ch. 7, Cramer Ch. 3)

Midterm.

Week 11, Mar. 22, Apr. 24.

Monte Carlo (Leach Ch. 8)

Week 12, Apr. 29, 31.

Free Energy Perturbation and Solvation (Leach Ch. 11, Cramer Chs. 11-12)

Week 13, Apr. 5, 7.

QM/MM (Cramer Chp. 13)

Week 14, Apr. 12, 14.

Finish working on term projects

Week 15, Apr. 19, 21.

Finish working on term projects

Week 16, Apr. 26, 28.

Study Day and Finals Week

Presentations of term projects

General Notes

Religious Holidays

Because of the extraordinary variety of religious affiliations of the University student body and staff, the Academic Calendar makes no provisions for religious holidays. However, it is University policy to respect the faith and religious obligations of the individual. Students with classes or examinations that conflict with their religious observances are expected to notify their instructors well in advance so that mutually agreeable alternatives may be worked out.

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Students who are registered with Student Disability Services and who are eligible for alternate testing accommodations such as extended test time and/or a distraction-reduced environment should present the required test permit to the professor at least one week in advance of the exam. Federal law requires that a student registered with SDS is entitled to the reasonable accommodations specified in the student's accommodation letter, which might include allowing the student to take the final exam on a day different than the rest of the class.

Academic Dishonesty -- Plagiarism and Cheating

*Academic misbehavior means any activity that tends to compromise the academic integrity of the institution or subvert the education process. All forms of academic misbehavior are prohibited at Wayne State University, as outlined in the Student Code of Conduct (<http://www.doso.wayne.edu/student-conduct-services.html>). Students who commit or assist in committing dishonest acts are subject to **downgrading** (to a failing grade for the test, paper, or other course-related activity in question, or for the entire course) and/or **additional sanctions** as described in the Student Code of Conduct.*

Cheating: Intentionally using or attempting to use, or intentionally providing or attempting to provide, unauthorized materials, information or assistance in any academic exercise. Examples include: (a) copying from another student's test paper; (b) allowing another student to copy from a test paper; (c) using unauthorized material such as a "cheat sheet" during an exam.

Fabrication: Intentional and unauthorized falsification of any information or citation. Examples include: (a) citation of information not taken from the source indicated; (b) listing sources in a bibliography not used in a research paper.

Plagiarism: To take and use another's words or ideas as one's own. Examples include: (a) failure to use appropriate referencing when using the words or ideas of other persons; (b) altering the language, paraphrasing, omitting, rearranging, or forming new combinations of words in an attempt to make the thoughts of another appear as your own.

Other forms of academic misbehavior include, but are not limited to: (a) unauthorized use of resources, or any attempt to limit another student's access to educational resources, or any attempt to alter equipment so as to lead to an incorrect answer for subsequent users; (b) enlisting the assistance of a substitute in the taking of examinations; (c) violating course rules as defined in the course syllabus or other written information provided to the student; (d) selling, buying or stealing all or part of an unadministered test or answers to the test; (e) changing or altering a grade on a test or other academic grade records.

Course Drops and Withdrawals *In the first two weeks of the (full) term, students can drop this class and receive 100% tuition and course fee cancellation. After the end of the second week there is no tuition or fee cancellation. Students who wish to withdraw from the class can initiate a withdrawal request on Pipeline. You will receive a transcript notation of WP (passing), WF (failing), or WN (no graded work) at the time of withdrawal. No withdrawals can be initiated after the end of the tenth week. Students enrolled in the 10th week and beyond will receive a grade. Because withdrawing from courses may have negative academic and financial consequences, students considering course withdrawal should make sure they fully understand all the consequences before taking this step. More information on this can be found at:*

<http://reg.wayne.edu/pdf-policies/students.pdf>