Syllabus

CHM4660/5660 - Computational Chemistry Fall 2016

Instructor: G. Andrés Cisneros 206C Chemistry
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Lectures: Mon, Wed 1:00 PM – 2:20 PM
Computational Chemistry Instructional Laboratory (CCIL)

Office Hours: Mon 3:00 – 4:00 PM or by appointment

The course will consist of lectures and hands-on computational labs. There will be one midterm (worth 30%), 7 computational assignments (33%), and a major computational project (35%). Midway through the semester you will submit a proposal for a final project. You should start thinking about your project as early as possible and discuss it with Prof. Cisneros.

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 AMBER16 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, 3rd. Ed., Gaussian Inc.
-"Molecular Modeling; 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: This department believes in reasonably accommodating individuals with disabilities and complies with the university policy established under Section 504 of the Rehabilitation Act of 1973 and the Americans with Disabilities Act (1990) to provide for equal access and opportunity. Please communicate with your professor as to your specific needs so appropriate arrangements can be made through the department and/or the Office of Disability Accommodation (Room 318A, University Union, (940) 565-4323).

Tentative Schedule:

Week 1, Aug 29, 31

Introduction to the course.
Population analysis and molecular properties, geometry optimization (Jensen Chs. 9-10)

Week 2, Sep 5, 7

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

Week 3, Sep. 12, 14

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

Week 4, Sep. 19, 21

Model chemistries, thermochemistry (Cramer Ch. 10)

Week 5, Sep 26, 28

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

Week 6, Oct. 3, 5

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

Week 7, Oct. 10, 12

Assorted special topics in electronic structure theory

Week 8, Oct. 17, 19

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

Proposals for term projects due

Week 9, Oct. 24, 26

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

Week 10, Oct. 31, Nov. 2

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

Midterm.

Week 11, Nov. 7, 9

Monte Carlo (Leach Ch. 8)

Week 12, Nov. 14, 16

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

Week 13, Nov. 21, 23

QM/MM (Cramer Chp. 13)

Week 14, Nov. 28, 30

Finish working on term projects

Week 15, Dec. 5, 7

Finish working on term projects

Week 16, Dec 12-15

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.

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 the University of North Texas, as outlined in the Student Code of Conduct (*https://policy.unt.edu/policydesc/university-north-texas-code-student-conduct-18-1-11*). *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 un-administered test or answers to the test; (e) changing or altering a grade on a test or other academic grade records.

Social Media Policies: Please see the document on the Blackboard site for this course (under "content")