Syllabus

CHM4660/5660 - Computational Chemistry Fall 2021

Instructor: G. Andrés Cisneros 205C Chemistry
e-mail: andres@unt.edu
Lectures: Mon, Wed 12:30 PM – 1:50 PM
Computational Chemistry Instructional Laboratory (CCIL)
Office Hours: Wed 10:00 – 11:00 AM or by appointment, all virtual

The course will consist of lectures and hands-on computational labs. There will be **one midterm (worth 30%)**, **7 computational assignments (35%)**, 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 Gaussian16 and AMBER21 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 will be reviewed. Additionally, students will become familiar with high performance computing (HPC) environments. The emphasis will be on 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).

INCLUSION & DIVERSITY: I value all students regardless of their background, country of origin, race, religion, ethnicity, disability status, etc., and am committed to providing a climate of excellence and inclusiveness within all aspects of the course. If there are aspects of your culture or identity that you would like to share with me as they relate to your success in this class, I am happy to meet to discuss. Likewise, if you have any concerns in this area or facing any special issues or challenges, you are encouraged to discuss the matter with me (set up a meeting by email) with an assurance of full confidentiality (only exception being mandatory reporting of academic integrity/code violations and/or sexual harassment).

Tentative Schedule:

Week 1, Aug 23, 25

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

Week 2, Aug 30, Sep 1

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

Week 3, Sep. 6 ***University Holiday, No Class***, 8

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

Week 4, Sep. 13, 15

Model chemistries, thermochemistry (Cramer Ch. 10)

Week 5, Sep 20, 22

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

Week 6, Sep 27, 29

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

Week 7, Oct. 4, 6

Assorted special topics in electronic structure theory

Week 8, Oct. 11, 13

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

Proposals for term projects due

Week 9, Oct. 18, 20

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

Midterm 10/20.

Week 10, Oct. 25, 27

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

Week 11, Nov. 1, 3

Monte Carlo (Leach Ch. 8)

Week 12, Nov. 8, 10

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

Week 13, Nov. 15, 17

QM/MM (Cramer Chp. 13)

Week 14, Nov. 22, 24

Finish working on term projects

Week 15, Nov. 29, Dec. 1

Finish working on term projects

Week 16, Dec 6, 8

Finals Week

Presentations of term projects

General Notes

Face Coverings

The North Texas region is currently experiencing high transmission of the highly contagious and dangerous Delta variant of COVID-19. The University of North Texas is very concerned about the risks of this new variant. UNT is requesting that all students, faculty and staff, whether vaccinated or not, comply with the public health recommendations of the U.S. Centers for Disease Control & Prevention in order to prevent Delta from spreading on campus. I ask that all students wear a mask during class and in other indoor locations on campus until we receive guidance that the public health risks have decreased significantly and no longer pose a threat. Masks will help us achieve our goal of protecting vulnerable members of the community and their families, including unvaccinated children, during this latest resurgence of COVID-19.

Read more about CDC guidelines for vaccinated people here:
https://www.cdc.gov/coronavirus/2019-ncov/vaccines/fully-vaccinated-guidance.html

Face covering guidelines could change based on community health conditions.

Attendance

Students are expected to attend class meetings regularly and to abide by the attendance policy established for the course. It is important that you communicate with the professor and the instructional team prior to being absent, so you, the professor, and the instructional team can discuss and mitigate the impact of the absence on your attainment of course learning goals. Please inform the professor and instructional team if you are unable to attend class meetings because you are ill, in mindfulness of the health and safety of everyone in our community.

If you are experiencing any symptoms of COVID-19 (https://www.cdc.gov/coronavirus/2019-ncov/symptoms-testing/symptoms.html) please seek medical attention from the Student Health and Wellness Center (940-565-2333 or askSHWC@unt.edu) or your health care provider PRIOR to coming to campus. UNT also requires you to contact the UNT COVID Team at COVID@unt.edu for guidance on actions to take due to symptoms, pending or positive test results, or potential exposure.

Course Materials for Remote Instruction

Remote instruction may be necessary if community health conditions change or you need to self-isolate or quarantine due to COVID-19. Students will need access to a webcam and microphone to participate in fully remote portions of the class. Information on how to be successful in a remote learning environment can be found at https://online.unt.edu/learn

Religious Holidays

Because of the extraordinary variety of religious affiliations of the University student body and staff, the Academic Calendar makes no provisions for almost any religious holidays. However, it is University policy to respect the faith and religious practices 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")

Legal Notice Regarding Lecture Notes

My lectures and notes are protected by state common law and federal copyright law. You are authorized to take notes in class thereby creating a derivative work from my lecture, but the authorization extends only to making one set of notes for your own personal use and no other use. You are not authorized to record my lectures, to provide your notes to anyone else (hard copy or electronic), or to make any other use of those notes without express prior written permission from me.

Email Use

My policy in this class is to **not** communicate any details regarding your grade through email. I will only discuss these details in person with a student.

Withdrawal from Class

The administration of this institution has set deadlines for withdrawal of any college-level courses. These dates and times are published in that semester's course catalog. Administration procedures must be followed. It is the student's responsibility to handle withdrawal requirements from any class. In other words, I cannot drop or withdraw any student. You must do the proper paperwork to ensure that you will not receive a final grade of "F" in a course if you choose not to attend the class once you are enrolled.

- **Last day to change your schedule without a "W" is Sep. 5**
- **Last day to drop with a "W" is Nov. 12**

Incomplete Grades

An "I" grade is a non-punitive grade given only during the last one-fourth of a semester and only if a student (1) is passing the course; (2) has justifiable reason why the work cannot be completed on schedule; and (3) arranges with the instructor to finish the course at a later date by completing specific requirements that the instructor must list on the electronic grade roster. All work in the course must be completed within the specified time (not to exceed one year after taking the course.) The last fourth of the current semester begins April 6.

Acceptable Student Behavior

Student behavior that interferes with an instructor's ability to conduct a class or other students' opportunity to learn is unacceptable and disruptive and will not be tolerated in any instructional forum at UNT. Students engaging in unacceptable behavior will be directed to leave the classroom and the instructor may refer the student to the Dean of Students to consider whether the student's conduct violated the Code of Student Conduct. The university's expectations for student conduct apply to all instructional forums, including university and electronic classroom, labs, discussion groups, field trips, etc. The Code of Student Conduct can be found at http://deanofstudents.unt.edu.

Emergency Notification and Procedures

UNT uses a system called Eagle Alert to quickly notify you with critical information in the event of an emergency (i.e., severe weather, campus closing, and health and public safety emergencies like chemical spills, fires, or violence). The system sends voice messages (and text messages upon permission) to the phones of all active faculty staff, and students. Please make certain to update your phone numbers at http://www.my.unt.edu. Some helpful emergency preparedness actions include: 1) know the evacuation routes and severe weather shelter areas in the buildings where your classes are held, 2) determine how you will contact family and friends if phones are temporarily unavailable, and 3) identify where you will go if you need to evacuate the Denton area suddenly. In the event of a university closure, please refer to Blackboard for contingency plans for covering course materials.

Retention of Student Records

Student records pertaining to this course are maintained in a secure location by the instructor of record. All records such as exams, answer sheets (with keys), and written papers submitted during the duration of the course are kept for at least one calendar year after course completion. Course work completed via the Blackboard online system, including grading information and comments, is also stored in a safe electronic environment for one year. You have a right to view your individual record; however, information about your records will not be divulged to other individuals without the proper written consent. You are encouraged to review the Public Information Policy and the Family Educational Rights and Privacy Act (FERPA) laws and the university's policy in accordance with those mandates at the following link: http://essc.unt.edu/registrar/ferpa.html

Student Perceptions On Teaching (SPOT)

Student feedback is important and an essential part of participation in this course. The Student Perceptions On Teaching (SPOT) is a requirement for all organized classes at UNT. This short survey will be made available at the end of the semester to provide you with an opportunity to evaluate how this course is taught. **Succeed at UNT**

UNT endeavors to offer you a high-quality education and to provide a supportive environment to help you learn and grown. And, as a faculty member, I am committed to helping you be successful as a student. Here's how to succeed at UNT: **Show up. Find Support. Get advised. Be prepared. Get involved. Stay focused.** To learn more about campus resources and information on how you can achieve success, go to http://success.unt.edu/

These descriptions and timelines are subject to change at the discretion of the Professor.