CHEM 4399/5399 Independent Study: Computational Chemistry
The University of Texas at Tyler, Spring 2025

Class Meeting Information
  MoWeFr 9:05AM - 10:00AM
  Ratliff Building South (RBS) 0**2019**
  01/13/2025 - 05/03/2025

Instructor Information
  Prof. Kai Zhang
  Office: RBS 3007A
  Phone: (903)566-6276
  Email: kzhang@uttyler.edu
  Office Hours: 10am-noon Monday and Wednesday,
                Noon-1pm Tuesday,
                and whenever I am in my office

Description
This course introduces students to the theoretical background and practical implementation of various computational chemistry methods, which may include ab initio self-consistent field (SCF) calculation, molecular mechanics force fields, Monte Carlo simulation, all-atom/coarse-grained molecular dynamics simulation and machine learning. Students will complete several computer projects using open-source packages on local computer facilities or remote servers. Pre-requisites: General Chemistry II or equivalent.

Learning Objectives
By the end of the course the students should be able to
  • Understand basic principles of molecular simulation across various time and length scales
  • Utilize popular simulation packages to perform computational tasks
  • Master scripting skills with Python
  • Interpret computational results in conjunction with experimental data

Required Textbook(s)
  None

Reference Textbook(s) and Materials
 [Cramer] *Essentials of Computational Chemistry: Theories and Models* by Christopher J Cramer
 ...

Other References and Reading Materials
Water Structure and Science https://water.lsbu.ac.uk/water/

Computer and software resources
Python https://education.molssi.org/python_scripting_cms/

Colab https://colab.research.google.com/
Avogadro https://avogadro.cc/
Molview https://molview.org/
VMD https://www.ks.uiuc.edu/Research/vmd/
WebMO https://www.webmo.net/
Martini http://www.cgmartini.nl/
GROMACS https://www.gromacs.org/
https://ringo.ams.stonybrook.edu/index.php/MD_Simulation:_Protein_in_Water
http://www.mdtutorials.com/gmx/

OpenMM https://openmm.org/

PDB https://www.rcsb.org/

LAMMPS https://www.lammps.org/
RDKit https://www.rdkit.org/
MDAnalysis https://www.mdanalysis.org/

Evaluation and Grade

Course work	%
Project(x8)	10% x 8 = 80%
Final Project	20%

The total number of points you attained on all graded work determines your final grade.

Grade	%
A	90 - 100
B	80 - 89
C	70 - 79
D	60 - 69
F	below 59

Topic Schedule (tentative)

Topic	Contents	Computer project
Week 1 Introduction to Python and Linux environment	Jupyter notebook Colab Numerical types Variable String Input/output Loop List/tuple/dictionary Function	Colab Python tutorial

Week 2 Computer Visualization	xyz file pdb file snapshot and animation images processing	matplotlib VMD Avogadro PyMOL XDrawChem
Week 3 Quantum Chemistry	Variational principle Born-Oppenheimer approximation Molecular orbital theory Basis sets expansions LCAO Many-electron wave functions Electron spin and antisymmetry Stater determinant Hartree-Fock self-consistent field (SCF) methods	
Week 4 Ab Initio Calculation I: Structures	Basis sets: Gaussian type and Slater type Close-shell and open-shell systems Single point energy Geometry optimization Charge distribution	ORCA WebMO Avogadro
Week 5 Ab Initio Calculation II: Properties	Rotation Vibration NMR spectral properties Zero-point energy Heat of formation?	ORCA WebMO Avogadro
Week 6 Review of Statistical Mechanics	Entropy Temperature Boltzmann distribution Free energy Partition function Ensemble Trajectory	
Week 7 Monte Carlo Simulation	Random number generator Uniform sampling Importance sampling Detailed balance Metropolis algorithm	Hard disks or hard spheres or Ising model?
Week 8 Numerical Differentiation and Integration	Trapezoidal rule Simpson's rule Gaussian quadrature Forward and backward differences Central difference Euler's method Runge-Kutta method	Python

Week 9 Molecular Dynamics of Simple Liquids	Newton's equation of motion Leapfrog method Verlet method Neighbor list Microcanonical ensemble (constant energy) simulation Constant temperature simulation with thermostat	Python MD simulation of Lennard-Jones liquids
Week 10 Molecular Mechanics	Bond stretching Bond angle bending Torsion Van der Waals forces Electrostatic forces Force field: Amber, CHARMM	
Week 11 All-Atom Molecular Dynamics Simulation	Protein folding/unfolding	GROMACS NAMD
Week 12 Coarse-Grained Model	united-atom model Bead-spring model for polymers FENE bond Martini force field	LAMMPS
Week 13 Introduction to Machine Learning	Supervised learning Classification and regression Loss function Gradient decent	scikit-learn
Week 14 Chemoinformatics	Fingerprint SMILES Graph representation	RDKit
Week 15 Neural Network and Deep Learning	Multilayer perceptron (MLP) Fully connected neural network Graph neural network Generative models	Keras
Week 16		

University Resources for Students
Resources to assist you in this course

- [UT Tyler Student Accessibility and Resource (SAR) OfficeLinks to an external site.](#) (provides needed accommodations to students with document needs related to access and learning)
- [UT Tyler Writing CenterLinks to an external site.](#)
- [The Mathematics Learning CenterLinks to an external site.](#)
- [UT Tyler PASS Tutoring CenterLinks to an external site.](#)
- [UT Tyler Supplemental InstructionLinks to an external site.](#)
- [Upswing (24/7 online tutoring) - covers nearly all undergraduate course areasLinks to an external site.Links to an external site.](#)
- [Robert Muntz LibraryLinks to an external site.](#) and [Library LiaisonLinks to an external site.](#)
- [Canvas 101Links to an external site.](#) (learn to use Canvas, proctoring, Unicheck, and other software)
- LIB 422 -- Computer Lab where students can take a proctored exam
- [The Career Success CenterLinks to an external site.](#)
- [UT Tyler Testing CenterLinks to an external site.](#)
- [Office of Research & Scholarship Design and Data Analysis LabLinks to an external site.](#)

Resources available to UT Tyler Students

- [UT Tyler Counseling Center Links to an external site.](#)(available to all students)
- [My SSP AppLinks to an external site.](#) (24/7 access to Student Support Program counseling through phone or chat and online wellness resources available in a variety of languages)
- [Student Assistance and Advocacy CenterLinks to an external site.](#)
- [Military and Veterans Success Center Links to an external site.](#)(supports for all of our military-affiliated students)
- [UT Tyler Patriot Food PantryLinks to an external site.](#)
- [UT Tyler Financial Aid and ScholarshipsLinks to an external site.](#)
- [UT Tyler Registrar's OfficeLinks to an external site.](#)
- [Office of International ProgramsLinks to an external site.](#)
- [Title IX ReportingLinks to an external site.](#)
- [Patriots EngageLinks to an external site.](#) (available to all students. Get engaged at UT Tyler.)

University Policies and Information

Withdrawing from Class

Students, you are allowed to [withdraw](#) (drop) from this course through the [Withdrawal Portal](#). Withdrawing from classes can impact Financial Aid, Scholarships, Veteran Benefits, Exemptions, Waivers, International Student Status, housing, and degree progress. Please read this page, speak with your instructors, consider your options, and speak with your instructor. UT Tyler faculty and staff are here for our students and often can provide additional support options or student assistance. Please read the implications for withdrawing from a course and the

instructions on using the Withdrawal portal on the Registrar's Withdrawal page.
Texas law prohibits students who began college for the first time in Fall 2007 or thereafter from dropping more than six courses during their entire undergraduate career. This includes courses dropped at other 2-year or 4-year Texas public colleges and universities. Consider the impact withdrawing from this class has on your academic progress and other areas, such as financial implications. We encourage you to consult your advisor(s) and financial aid for additional guidance. CAUTION #1: Withdrawing before census day does not mean you get a full refund. Please see the Tuition and Fee Refund Schedule. CAUTION #2: All international students must check with the Office of International Programs before withdrawing. All international students are required to enroll full-time for fall and spring terms. CAUTION #3: All UT Tyler Athletes must check with the Athletic Academic Coordinator before withdrawing from a course. CAUTION #4: All veterans or military-affiliated students should consult with the Military and Veterans Success Center.

Final Exam Policy

Final examinations are administered as scheduled. If unusual circumstances require that special arrangements be made for an individual student or class, the Dean of the appropriate college, after consultation with the faculty member involved, may authorize an exception to the schedule. Faculty members must maintain student final examination papers for a minimum of three months following the examination date.

Incomplete Grade Policy

If a student, because of extenuating circumstances, is unable to complete all of the requirements for a course by the end of the semester, then the instructor may recommend an Incomplete (I) for the course. The "I" may be assigned in place of a grade only when all of the following conditions are met: (a) the student has been making satisfactory progress in the course; (b) the student is unable to complete all coursework or final exam due to unusual circumstances that are beyond personal control and are acceptable to the instructor, and (c) the student presents these reasons before the time that the final grade roster is due. The semester credit hours for an Incomplete will not be used to calculate the grade point average. The student and the instructor must submit an Incomplete Form detailing the work required and the time by which the work must be completed to their respective department chair or college dean for approval. The time limit established must not exceed one year. Should the student fail to meet all of the work for the course within the time limit, then the instructor may assign zeros to the unfinished work, compute the course average for the student, and assign the appropriate grade. If a grade has yet to be assigned within one year, then the Incomplete will be changed to an F, or NC. If the course was initially taken under the CR/NC grading basis, this may adversely affect the student's academic standing.

Grade Appeal Policy

Disputes regarding grades must be initiated within sixty (60) days from the date of receiving the final course grade by filing a Grade Appeal Form with the instructor who assigned the grade; this is separate from the Application for Appeal form submitted to the Student Appeals Committee, which does not rule on grade disputes as described in this policy. If the student is not satisfied with the decision, the student may appeal in writing to the Chairperson of the

department from which the grade was issued. In situations where there is an allegation of capricious grading, discrimination, or unlawful actions, appeals may go beyond the Chairperson to the Dean of the college from which the grade was issued, with that decision being final. The Grade Appeal form is found in the Registrar's Form Library.

Disability/Accessibility Services

In accordance with Section 504 of the Rehabilitation Act, Americans with Disabilities Act (ADA) and the ADA Amendments Act (ADAAA), the University of Texas at Tyler offers accommodations to students with learning, physical, and/or psychological disabilities. If you have a disability, including a non-visible diagnosis such as a learning disorder, chronic illness, TBI, PTSD, ADHD, or a history of modifications or accommodations in a previous educational environment, you are encouraged to visit https://hood.accessiblelearning.com/UTTyler and fill out the New Student application. The Student Accessibility and Resources (SAR) office will contact you when your application has been submitted and an appointment with the Assistant Director Student Accessibility and Resources/ADA Coordinator. For more information, including filling out an application for services, please visit the SAR webpage at https://www.uttyler.edu/disability-services, the SAR office located in the University Center, # 3150, or call 903.566.7079."

Military Affiliated Students

UT Tyler honors the service and sacrifices of our military-affiliated students. If you are a student who is a veteran, on active duty, in the reserves or National Guard, or a military spouse or dependent, please stay in contact with your faculty member if any aspect of your present or prior service or family situation makes it difficult for you to fulfill the requirements of a course or creates disruption in your academic progress. It is important to make your faculty member aware of any complications as far in advance as possible. Your faculty member is willing to work with you and, if needed, put you in contact with university staff who are trained to assist you. The Military and Veterans Success Center (MVSC) has campus resources for military-affiliated students. The MVSC can be reached at MVSC@uttyler.edu or via phone at 903.565.5972.

Students on an F-1 Visa

To remain in compliance with Federal Regulations requirements you must do the following:

- Traditional face-to-face classes: Attend classes on the regular meeting days/times.
- Hybrid Classes:Attend all face-to-face classes convened by the instructor and meet with the Office of International Programs according to the schedule set for your specific course.
- Online course: Only one online course can count toward your full-time enrollment. Students are expected to be fully engaged and meet all requirements for the online course.

Academic Honesty and Academic Misconduct

The UT Tyler community comes together to pledge that "Honor and integrity will not allow me to lie, cheat, or steal, nor to accept the actions of those who do." Therefore, we enforce

the Student Conduct and Discipline policy in the Student Manual Of Operating Procedures (Section 8).

FERPA

UT Tyler follows the Family Educational Rights and Privacy Act (FERPA) as noted in University Policy 5.2.3. The course instructor will follow all requirements to protect your confidential information.

Absence for Official University Events or Activities

This course follows the practices related to approved absences as noted by the Student Manual of Operating Procedures (Sec. 1 -501).

Absence for Religious Holidays

This course follows the practices related to Excused Absences for Religious Holy Days as noted in the Catalog.

Campus Carry

We respect the right and privacy of students who are duly licensed to carry concealed weapons in this class. License holders are expected to behave responsibly and keep a handgun secure and concealed. More information is available at http://www.uttyler.edu/about/campus-carry/index.php.