Course Syllabus

Course Information

Course Prefix, Number, Section	*CHEM 6V39*
Course Title	*Special Topics in Organic Chemistry: Computational Chemistry & Reaction Mechanisms*
Term	*Fall 2025*
Days & Times	*TR, 4:00 pm – 5:15 pm, SLC 2.203*

Professor Contact Information

Professor	*Dr. Alistair J. Sterling*
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Office Location	*BSB 11.431*
Office Hours	*TBA*

Course Pre-requisites, Co-requisites, and/or Other Restrictions

Consent of instructor required

Course Description

This course will cover the essentials to enable students to understand and use a range of computational methods for molecular simulations. Students will calculate molecular properties, and model organic and organometallic reactions. A range of approaches will be covered, including DFT and machine learning. Graduate students will carry out a short computational study, and write up, present and peer-review it in the style of a conference for the final grade.

Student Learning Objectives/Outcomes

1. Students will learn how to form a computational hypothesis.
2. Students will learn the essentials of quantum chemistry that enable the best choice of method for the property or mechanism at hand.
3. Students will learn how to connect computations to experimental reality using transition state theory and physical organic chemistry principles.
4. Students will learn how and when to use machine learning and artificial intelligence tools to study molecules and chemical reactions.
5. Students will learn to critically analyze the primary computational chemistry literature.
6. Students will demonstrate how computational techniques can be used to study molecular problems (graduate-level course project to be presented as a final exam).

Required Textbooks and Materials

Required Texts
None

Required Technology
A Mac/Windows/Linux laptop will be required for some exercises and for the final graduate student presentation. Please discuss access to a laptop with the Instructor if there are any issues.

Suggested Course Materials

Suggested Readings/Texts
Computational Chemistry (Oxford Chemistry Primer series), Jeremy Harvey (*ISBN: 9780198755500*)

Modern Physical Organic Chemistry, Anslyn & Doherty (*ISBN: 978-1-891389-31-3, eISBN: 978-1-891389-48-1*)

Modern Quantum Chemistry, Szabo & Ostlund (*ISBN: 9780486691862*)

Introduction to Computational Chemistry (3rd edition), Jensen (*ISBN: 978-1-118-82599-0*)

Essentials of Computational Chemistry: Theories and Models (2nd edition), Cramer (*ISBN: 978-0-470-09182-1*)

Suggested Readings/Texts
Selected material will be provided by the Instructor during the course

Assignments & Academic Calendar

Topics, Reading Assignments, Due Dates, Exam Dates

Week 1	Introduction to computational chemistry
Week 2	Electronic structure theory: The machinery of quantum chemistry
Week 3	Electronic structure theory: Basis sets
Week 4	Electronic structure theory: Hartree-Fock theory
Week 5	Electronic structure theory: Post-Hartree Fock methods and DFT
Week 6	Connecting computations to experimental reality: Solvation and thermodynamics
Week 7	Connecting computations to experimental reality: Thermodynamics properties and transition state theory
Week 8	Review session and Graduate midterm
Week 9	Computing properties of chemical systems: Distortion/interaction analysis, energy decomposition analysis, and excited states
Week 10	Computing properties of chemical systems: Electronic properties
Week 11	Data-driven chemistry: Theoretical physical organic chemistry
Week 12	Data-driven chemistry: Machine learning and artificial intelligence
Week 13	Individual project work

Week 14 **Fall Break**

Week 15 Final exam presentations

Week 16 Final exam presentations

Mid-term exam: October 16th

Final exam: December 2nd (Group 1), December 4th (Group 2), December 9th (Group 3)

Grading Policy

Problem sets (20%), graduate midterm exam (20%), final individual project presentation (30%), final individual project report/peer-review, including critical analysis/review of the primary literature (20%), active participation in final exam presentations (10%).

Course Policies

Make-up exams

There will be no make-up exams except for documented circumstances.

Extra Credit

None

Late Work

No late work will be accepted except for documented circumstances

Special Assignments

In-class student presentations, written assignments and instructions will be provided to the students during the course.

Comet Creed

This creed was voted on by the UT Dallas student body in 2014. It is a standard that Comets choose to live by and encourage others to do the same:

"As a Comet, I pledge honesty, integrity, and service in all that I do."

Academic Support Resources

The information contained in the following link lists the University's academic support resources for all students.

Please see http://go.utdallas.edu/academic-support-resources.

UT Dallas Syllabus Policies and Procedures

The information contained in the following link constitutes the University's policies and procedures segment of the course syllabus.

Please go to http://go.utdallas.edu/syllabus-policies for these policies.

The descriptions and timelines contained in this syllabus are subject to change at the discretion of the Professor.