WISCONSIN
UNIVERSITY OF WISCONSIN–MADISON

Topics in Computational: Chemistry 635
Credits: 1
Canvas Course URL: https://canvas.wisc.edu/courses/90992

Meeting Time and Location: T Th 9:55 am
Room 1381 Chemistry (GradLab)

Instructional Mode*:*
This class meets one 50-minute class period each week over the fall/spring semester and carries the expectation that students will work on course learning activities (reading, writing, problem sets, studying, etc) for about 2 hours out of the classroom for every class period. The syllabus includes additional information about meeting times and expectations for student work.

INSTRUCTOR:

Dr. Desiree Bates Computational Chemistry Leader
Instructor Availability
Office Hours: By appointment only

Instructor Email/Preferred Contact: 9307 Chemistry
(608) 262-6936
dmbates@chem.wisc.edu (preferred)

OFFICIAL COURSE DESCRIPTION

Topics in Computational Chemistry is a semester long course designed to initiate and facilitate computational methods for students with little to no background on the topic. While doing so, we will explore a variety of software packages including different visualization software. Students will learn basic calculations and have example inputs and outputs for future use. We will evaluate outputs and interpret error messages. In addition, we will discuss different methodologies for various chemical systems. Finally, we will explore the literature and understand basic ways of writing computational methodologies and findings.
Requisites: Graduate Standing

LEARNING OUTCOMES

*   Students will have a basic knowledge of computational chemistry.
*   Student will be able to perform basic computations with a variety of software.
*   Students will be able to design their own computational experiments.
*   Students will examine technical literature, resolve ambiguity and develop conclusions.

GRADING

This course is credit/no credit. Credit is determined by the following:
- In class attendance: Students may only miss one class. Missing more than one lecture will automatically yield no credit for the course.
- Assignments: Students must turn in all assignments before the class scheduled final. All assignments will be graded and returned to students. If the assignment/calculation is not preformed correctly, students will need to resubmit assignments.

REQUIRED TEXTBOOK, SOFTWARE & OTHER COURSE MATERIALS

An active Sunbird cluster account. To obtain one just email:
clusteradmin@chem.wisc.edu

COURSE DESIGNATIONS: Advanced level; physical science breadth; counts as L&S credit.

HOMEWORK & OTHER ASSIGNMENTS

- Homework consist of computations and an accompanying handout to be turned in for verification of correctly completed results.

TENTATIVE COURSE OUTLINE:

Week	Topic	
1	Introduction to Computational Chemistry	
	What is a potential energy surface?	Using WebMO: 1 dimensional scan.
2	Locating a minima energy structure: Geometry Optimization	Using WebMO: Building a geometry optimization input for Gaussian Software.
	Determining the nature of a stationary point: Harmonic Vibrational Frequency	Using WebMO: Building an input for a frequency calculation
3	Trouble Shooting an optimization	Using WebMO: Using force constants to optimize a difficult structure
	Transition States	Using WebMO: Optimizing a transition state
4		Using WebMO: QST2/QST3 calculations
	Reaction Pathways	Using WebMO:

		IRC calculation
5	Thermodynamic Quantities	Using WebMO: Enthalpy of a reaction
6	Single-point energies	Using WebMO: Relative energies of isomers
	Relative energies	
7	Excited State Calculations	Using WebMO: UV-VIS
		Using WebMO: Electron Affinities; Koopman's Theorem
8	Convergent Methods	Using WebMO: Quantum Mechanical Calculations
	Hartree-Fock & MPn Theories	Using WebMO: Single Point Energies
9	No class: Spring Break	
10	Coupled Cluster Theory	Using WebMO: CCSD(T) energy
	Basis Sets	Using WebMO: Comparing results with various basis set calculations
11	Basis sets	
	Density Functional Theory	Using WebMO: DFT energies
12	Natural Bond Orbitals	Using WebMO: Interpret the NBOs for various systems
	Basic Shell Commands, queue commands, and accessing phoenix	Building directories, basic file managing, and understanding queues
13	VI text editor	Creating basic input files without using WebMO
	Gaussian input file structure	
14	Other software Packages	CFOUR, MOLPRO and ORCA
15	Molecular Mechanics	Using Gromacs Software Molecular Dynamics Simulations
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ACADEMIC INTEGRITY

By enrolling in this course, each student assumes the responsibilities of an active participant in UW-Madison's community of scholars in which everyone's academic work and behavior are held to the highest academic integrity standards. Academic misconduct compromises the

integrity of the university. Cheating, fabrication, plagiarism, unauthorized collaboration, and helping others commit these acts are examples of academic misconduct, which can result in disciplinary action. This includes but is not limited to failure on the assignment/course, disciplinary probation, or suspension. Substantial or repeated cases of misconduct will be forwarded to the Office of Student Conduct & Community Standards for additional review. For more information, refer to studentconduct.wiscweb.wisc.edu/academic-integrity/.

ACCOMMODATIONS FOR STUDENTS WITH DISABILITIES

McBurney Disability Resource Center syllabus statement: "The University of Wisconsin-Madison supports the right of all enrolled students to a full and equal educational opportunity. The Americans with Disabilities Act (ADA), Wisconsin State Statute (36.12), and UW-Madison policy (Faculty Document 1071) require that students with disabilities be reasonably accommodated in instruction and campus life. Reasonable accommodations for students with disabilities is a shared faculty and student responsibility. Students are expected to inform faculty [me] of their need for instructional accommodations by the end of the third week of the semester, or as soon as possible after a disability has been incurred or recognized. Faculty [I], will work either directly with the student [you] or in coordination with the McBurney Center to identify and provide reasonable instructional accommodations. Disability information, including instructional accommodations as part of a student's educational record, is confidential and protected under FERPA." http://mcburney.wisc.edu/facstaffother/faculty/syllabus.php

DIVERSITY & INCLUSION

Institutional statement on diversity: "Diversity is a source of strength, creativity, and innovation for UW-Madison. We value the contributions of each person and respect the profound ways their identity, culture, background, experience, status, abilities, and opinion enrich the university community. We commit ourselves to the pursuit of excellence in teaching, research, outreach, and diversity as inextricably linked goals.

The University of Wisconsin-Madison fulfills its public mission by creating a welcoming and inclusive community for people from every background – people who as students, faculty, and staff serve Wisconsin and the world." https://diversity.wisc.edu/