Topics in Computational Chemistry 635 Spring 2020

Lecture:	TTh 9:55 am Room 1381 Chemistry
Lecturer:	Dr. Desiree Bates 9307 Chemistry (608) 262-6936 dmbates@chem.wisc.edu
Office Hours:	By appointment only

Class 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. This course does not fulfill any requirements for any degrees.

Suggested Books
Exploring Chemistry with Electronic Structure Methods Third Edition by James B. Foresman and AEleen Frisch.

Essentials of Computational Chemistry 2nd edition: Theories and Models by Christopher Cramer.
ISBN 978-0-470-09182-1

Lectures
You are expected and required to attend all lectures. Because this is a one-credit course, all of the material will be covered in lecture with little outside work. In addition, valuable calculations will be performed during lecture and are vital to the understanding and success of this course.

Grading
This course will be a credit/no credit course. *Students are allowed to miss one lecture.* Missing more than one lecture will automatically yield no credit for the course. In addition, students must complete the in class calculations for credit for the course.

Students with Disabilities
Appropriate accommodations for this course can be arranged for students with disabilities. If you are a student with physical, learning, emotional, or psychological disabilities, you are encouraged to make an appointment with McBurney Disability Resource Center for

assistance. http://www.mcburney.wisc.edu. Please schedule a confidential meeting with Dr. Bates as soon as possible to discuss arrangements for your learning.

Academic Misconduct

Academic honesty is essential to the existence and integrity of an institution of higher education. The responsibility for maintaining that integrity is shared by all members of the academic community. Thus, academic misconduct will not be tolerated at this University. Any student caught cheating or attempting to cheat will be punished by automatically receiving a zero for that assignment. Academic misconduct includes copying from another's assignment, plagiarizing published materials and/or fabricating results. A second infraction will result in a failure for the course. Refer to the UW academic polices for more information on what constitutes academic misconduct. http://www.wisc.edu/students/saja/misconduct/UWS14.html

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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