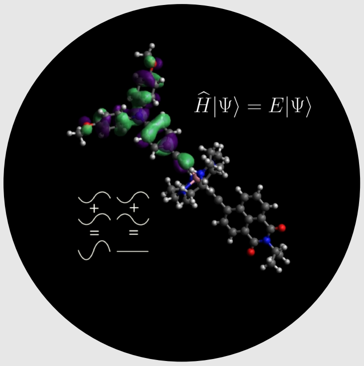

Molecular Simulation

CHEM 590 (Spring 2020)

Instructor Info

Prof. David N. Beratan

david.beratan@duke.edu

Course Info

Prereq: Physical Chemistry or equivalent.

Tues & Thurs

4:40-5:55PM

Classroom: FFSC 2237

TAs Info

Jesús Valdiviezo

Office Hrs: Tu & Th 3:30-4:30PM

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Jonathon Yuly

Office Hrs: Tu & Th 2:30-3:30PM

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Overview

This is a flipped course designed to introduce students to the interdisciplinary aspects of molecular simulation by integrating important components of several research fields. This integrated approach will cross the traditional disciplines of Chemistry, Physics and Biology.

Upon completion of this course, students will be able to use computational tools to predict molecular properties and simulate systems of biological interest. They will also have a fundamental knowledge of the theory behind electronic structure calculations and molecular dynamics simulations.

Material

Primary Materials

Cramer, Christopher J. Essentials of computational chemistry: theories and models. John Wiley & Sons, 2004 (Cramer).

Recommended Texts and Resources

Koch, Wolfram, and Max C. Holthausen. A chemist's guide to density functional theory. John Wiley & Sons, 2001 (Koch).
Piela, Lucjan. Ideas of quantum chemistry. Elsevier, 2013 (Piela).
Jensen, Jan H. Molecular modeling basics. CRC Press, 2010 (Jensen).
Lecture Materials from Prof. Christopher Cramer at UMN.
(http://pollux.chem.umn.edu/8021/Lectures/)

Other

Lecture notes, selected input files, journal articles and book chapters will be provided on Sakai.

Software

Gaussian	https://www.gaussian.com
NAMD	https://www.ks.uiuc.edu/Research/namd/
Avogadro	https://avogadro.cc/
Gabedit	http://gabedit.sourceforge.net/
VMD	https://www.ks.uiuc.edu/Research/vmd/
MarvinSketch	https://chemaxon.com/products/marvin
ChemDraw	https://software.duke.edu/node/49
MATLAB	https://software.duke.edu/node/130

Grading Scheme

20%	In-Class Worksheets
20%	Homework
25%	Project I (15% Report, 10% Presentation)
35%	Project II (25% Report, 10% Presentation)

FAQs

Do I need to know how to code?

Not necessarily. During the course you will learn some code basics and how to apply them to molecular simulation. If you are more interested in coding you can apply your skills on the course projects.

My math background is not strong, but I want to learn more about molecular simulation, Is this course for me?

Yes it is! Don't worry too much about the derivations. Although we'll see several equations, what is most important in this course is to understand the concepts and to interpret the simulation results.

Do I need to bring my computer to all sessions?

Yes, we will do active learning in class, so you would require to have your computer to run simulations. If you're unable to bring your computer to a session let us know in advance and we could provide you one.

Can I work on a particular problem/challenge from my research group for the final project?

Yes, and we encourage you to work on projects that you are passionate about.

Course Target Audience

This course is for anyone who wants to learn molecular simulation tools. As a graduate-level course it will help Ph.D. students to incorporate molecular simulation in their research endeavors. Undergraduate students interested in learning research skills and reviewing fundamental concepts of molecules and materials are also welcomed.

Learning Objectives

- Become familiar with the current simulation tools for molecules and materials.
- Improve your understanding of the basic physics behind molecular simulation.
- Learn to conduct an original research project and present research results.

Projects

Students will choose and study molecular systems or materials of interest and apply some of the computational tools covered in class. Some proposed projects will be listed on Sakai, but students are encouraged to proposed their own projects.

Communication

All questions on homework, projects, lectures, etc. should be posted to Piazza for open discussion. It is OK for the post to be kept as "anonymous." If students email the professor or TAs with questions on the homework or lecture, they will likely be asked to post the question to Piazza to be answered there for the entire class to access.

Sign-up Link: `https://piazza.com/duke/spring2020/chem59002sp20`

Class Link: `https://piazza.com/duke/spring2020/chem59002sp20/home`

Attendance and Make-up Policy

Attendance to the lectures is crucial to succeeding in this course. Homework will be due each week or two weeks and must be turned in at the beginning of class – make-up assignments will only be allowed for students who have a substantiated excuse approved by the instructor *before the due date*.

Diversity and Inclusivity Statement

We consider this classroom to be a place where you will be treated with respect, and we welcome individuals of all ages, backgrounds, beliefs, ethnicities, genders, gender identities, gender expressions, national origins, religious affiliations, sexual orientations, ability - and other visible and non-visible differences. All members of this class are expected to contribute to a respectful, welcoming and inclusive environment for every other member of the class.

Collaboration Policy

Students are allowed to work together on homework, keeping in mind that the Duke Community Standard (`https://integrity.duke.edu/`) applies to all assignments. Each student must personally work each problem, legibly write up and submit their own solutions.

Academic Integrity

Academic integrity is expected as part of the community to which you belong and each student will be held accountable for upholding the standard. University policy will be enforced in the case of any dishonest conduct.

Lecture Schedule

Part 1: The Main Tools of Electronic Structure Calculations

Jan 9	Introduction and course overview	Frenkel, Daan, and Berend Smit. Understanding molecular simulations: from algorithms to applications. Academic press, 2002. Ch. 1, pp. 1-6
	Hands–on activities: Installation of software packages, class survey.	
Jan 14	Postulates of Quantum Mechanics	Piela Ch.1 (pp 15-36)
	Introduction to cluster computing	Lecture notes
	Hands–on activities: Communicating with the clusters, UNIX commands, introduction to SLURM.	
Jan 16	Molecular hamiltonians	Cramer Ch. 4
	The Born-Oppenheimer approximation	
	Single point calculations	
	Hands–on activities: Using Avogadro, charge and dipole moment calculations.	
Jan 21	Potential energy surfaces	Jensen Ch. 1
	Force fields	Cramer Ch. 2
	Molecular dynamics basics	
	Hands–on activities: Potential energy surface scans and vibrational motions.	
Jan 23	The variational principle	Piela Ch. 5 (pp 231-253)
	Self-consistent approach	
	Hands–on activities: Calculate molecules in singlet and triplet ground states.	
Jan 28	Hartree-Fock	Cramer Ch. 6
	Hands–on activities: Calculate vibrational spectra and thermodynamic properties.	
Jan 30	Hartree-Fock cont.	
	Basis sets	
	Hands–on activities: Calculate orbital energies, plotting orbitals.	
Feb 4	Electron correlation methods	Cramer Ch. 7
	Hands–on activities: Comparison of results of ab initio methods.	
Feb 6	Electron correlation methods cont.	
	Hands–on activities: Calculation of excited states of conjugated molecules with CIS.	
Feb 11	Density functional theory	Cramer Ch. 8
	Hands–on activities: Reaction intermediates and transition states.	

Feb 13	Density functional theory cont.	Koch Ch. 5
	Hands–on activities: Calculate inorganic complexes using ECPs.	

Part 2: Specialized Tools of Electronic Structure Calculations

Feb 18	Excited states (TD–DFT)	Cramer Ch. 14 Adamo, Carlo, and Denis Jacquemin. "The calculations of excited-state properties with Time-Dependent Density Functional Theory." Chemical Society Reviews 42, no. 3 (2013): 845-856
	Hands–on activities: Calculate UV-Vis spectra of organic and inorganic molecules.	
Feb 20	Solvation effects	Cramer Ch. 11
	Hands–on activities: Calculation of solvation energies and excited state properties with implicit solvent.	
Feb 25	PROJECT I PRESENTATIONS DAY 1	
	Hands–on activities: Presenters will walk us through the calculations performed.	
Feb 27	PROJECT I PRESENTATIONS Day 2	
	Hands–on activities: Presenters will walk us through the calculations performed.	
March 3	Dispersion effects and error correction methods	Lecture notes
	Hands–on activities: Case studies were corrections are needed.	
March 5	Charge and energy transfer	Lecture notes
	Hands–on activities: Calculate donor–bridge–acceptor systems and electronic couplings. PROJECT II PROPOSALS DUE	
March 10	No class (spring recess)	
March 12	No class (spring recess)	

Part 3: Molecular Dynamics Simulations

March 24	Introduction to molecular dynamics	Frenkel Ch 2 Frenkel Ch 4 (pp 63-74)
	Hands–on activities: Perform molecular dynamics simulation of a small ligand	
March 26	Structure preparation for molecular dynamics	Notes from Beratan Lab members
	Hands–on activities: Preparation of a protein crystal structure for molecular dynamics simulations.	
March 31	Molecular dynamics of biomolecules	Cramer. Ch. 3
	Hands–on activities: Simulation of a biological molecule using molecular dynamics.	

April 2	Dynamics, sampling and kinetics	Lecture notes from TSTC 2019
	Hands–on activities: Analyze trajectories of molecular dynamics simulations.	
April 7	Free energies in small molecules	Lecture notes from TSTC 2019 Cramer Ch. 12
	Hands–on activities: Calculation of ligand-protein binding free energy	
April 9	Free energies in large molecules	Lecture notes from TSTC 2019
	Hands–on activities: Calculation of ligand-protein binding free energy	
April 14	PROJECT II PRESENTATIONS	
	Hands–on activities: Groups will walk us through the calculations performed.	