Computational Chemistry

Chemistry 438/550, Spring 2021

Instructor: Prof. Lu Wang **Email:** lwang@chem.rutgers.edu

Lectures: Tuesday and Thursday 9:15 – 10:35 am

Online classes:
https://rutgers.zoom.us/j/98648983131?pwd=Z0xOcWVlV3hXdnlocDUzZFBFVXlTZz09

Passcode: CompClass

Office Hour: Friday 2 – 3 pm or by appointment. Use the above link for the meetings.

Text: Christopher J. Cramer, "Essentials of Computational Chemistry: Theories and Models, Second Edition", Wiley

Recommended reading:

James Foresman and Aleen Frisch "Exploring Chemistry with Electronic Structure Methods", Gaussian Inc.

Daan Frenkel and Berend Smit, "Understanding Molecular Simulation, From Algorithms to Applications", Academic Press

Amber tutorials: https://ambermd.org/tutorials/

Course Description: This course will provide theoretical background and practical guidelines for using computational methods such as electronic structure calculations and classical molecular mechanics simulations in solving chemical and biological problems. The course will acquaint the students with the wide variety of computational tools available for molecular modeling and simulations, and provide them with practical examples for using software packages Gaussian and Amber.

Grading: Homework assignments 60%

Final project 40%

Homework: Electronic or scanned copy submitted through the course canvas site.

Final project: Every student will perform computer simulations for a chemical or biological system, preferably related to their own research. Grading of the final project will be based on both the written report and oral presentation. The report should be 3-10 pages, which describes the purpose of the study, the system studies, the methods used and the results

obtained. The oral presentation will be 10 minutes for each student. Students should submit an initial proposal of the final project by March 12th. The initial proposal should include a few sentences about the motivation of your simulations, the systems you will simulate and the methods you will use in the simulations.

Class Schedule

Date	Topic	Recommended reading
Jan 19	Introduction to computational chemistry	Textbook: Chapter 1
Jan 21	Molecular orbital theory	Textbook: 4.1-4.4
Jan 26	Many-electron wave functions	Textbook: 4.5
Jan 28	Hartree-Fock theory	Textbook: 4.5.5, 6.3.3
Feb 2	Basis sets	Textbook: 6.2
Feb 4	Introduction to Gaussian and GaussView	Comp practice
Feb 9	Electron correlations	Textbook: Chapter 7
Feb 11	Geometry optimization and frequency calculations	Comp practice
Feb 16	Density functional theory	Textbook: Chapter 8
Feb 18	Charge distributions and spectroscopy properties	Textbook: Chapters 9-11 Comp practice
Feb 23	Thermodynamic properties, reaction transition state	
Feb 25	Implicit models for condensed phases	
March 2	Overview of statistical mechanics, ensembles	Textbook: 3.1-3.2
March 4	Force fields	Textbook: 2.2
March 9	Monte Carlo simulations	Textbook: 3.4
March 11	Molecular dynamics simulations	Textbook: 3.3
March 16, 18	**No class, Spring Recess**	
March 23	Introduction to Amber16, set up for liquid water simulations	Textbook: 3.5 Comp practice
March 25	Liquid water simulations – properties	
March 30	Free energy calculations – alanine dipeptide	Tutorial Comp practice
April 1	Free energy calculations – enhanced sampling	
April 6	Free energy calculations – free energy perturbation and thermodynamic integration	Textbook: 12.2
April 8	Example of protein free energy calculations – setting up the system	Tutorial Comp practice
April 13	Example of protein free energy calculations – analyze the results	
April 15	Systems without a force field – example simulations of ionic liquids	Tutorial Comp practice

April 20	QM/MM methods	Textbook: Chapter 13
April 22	Guest lecture, Dr. David Cerutti	
April 27	Final project presentations	
April 29	Final project presentations	
April 30	Final project presentations	
May 5	Written report due	