Computational Chemistry

Chemistry 438/550, Fall 2022

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

Lectures: Tuesday and Thursday 3:50 – 5:10 pm, CCB-1203

Office Hour: Friday 10 – 11 am or by appointment

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 Oct 28th. 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.

Academic Integrity: All University policies on academic integrity will be strictly enforced. Any cheating on quizzes, exams, or other assignments will be treated promptly in strict accordance with the Rutgers University Academic Integrity Policy. A copy of the current Academic Integrity Policy, which went into effect on September 1, 2013, can be found at

https://slwordpress.rutgers.edu/academicintegrity/wp-content/uploads/sites/41/2014/11/AI_Policy_2013.pdf

Please read the policy carefully if you are not familiar with it.