

Chemistry 438/550: Computational Chemistry

David Case, instructor. Office: 208b Proteomics, phone: 848-445-5885; cell: 609-751-8668

email: david.case@rutgers.edu

Spring 2020, Mondays and Wednesdays, noon to 1:20pm, CCB 1203

This is a one-semester physical chemistry course, covering the theory and practice of computational explorations in chemistry and biochemistry. You should have completed undergraduate physical chemistry, such as CCB 327/328 or 341/342 here at Rutgers. This course will provide theoretical background and practical guidelines for using computational methods, especially electronic structure calculations and classical molecular mechanics simulations, in studying chemical and biological systems. It will acquaint students with a variety of computational tools available for molecular modeling and simulation, and provide them with practical examples for using several software packages, including Gaussian and Amber.

The course text is Christopher J. Cramer, *Essentials of Computational Chemistry: Theories and Models, Second Edition*, (Wiley). There will be additional handouts for most topics. The table below gives an approximate time schedule; detailed reading assignments will be made as the class proceeds.

Week starting	Subject	Chapter
Jan 22, 27	Computational basics: the command-line, shells, AWK	
Feb 3	Working with data: relational databases	
Feb 10, 17	Molecular orbital theory and practice	1,4-6
Feb 24	Electron correlation, density functional theory	7-8
Mar 2,9	Spectroscopy and excited states	9,10,14
Mar 23, 30	Molecular mechanics and dynamics	2,3,12
Apr 6	Condensed phases, connections to thermodynamics	11,15
Apr 13, 20	Biomolecular simulations; connections to experiment	
Apr 27, May 4	Student project presentations	

The course website is <http://casegroup.rutgers.edu/lnotes.html>. Reading and homework assignments and additional course materials will be posted there. Final grades in the class will be based on assigned homework/problem sets (60%), and projects/presentations (40%). Midway through the semester, each student will choose a project, which can be related to research you are carrying out, or to some facet of computational chemistry that interests you. Students will be expected to make a short oral presentation to the rest of the class, as well as to attend and provide feedback to other student presentations. A written summary of the project will also be required.

Please note: Students are expected to adhere the university policies on academic integrity and student conduct in all assignments, assessments and other matters regarding this course. These policies can be found online: <http://studentconduct.rutgers.edu/academic-integrity/>. You may consult with fellow students on homework and on class projects, but you must personally prepare and understand any written material you hand in. You may *not* consult with fellow students on the final project.