Chemistry 438/550: Computational Chemistry

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Spring 2022, Mondays and Thursdays, 8:30 to 9:50am, CCB 1209

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 here at Rutgers or the equivalent elsewhere. 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 Frank Jensen, *"Introduction to Computational Chemistry, Third Edition"*, (Wiley). There will be additional handouts for many topics. The table below gives an approximate time schedule; detailed reading assignments will be made as the class proceeds.

Week starting	**Subject**	**Chapter**
Jan 20, 24, 31	Computational basics: the command-line, shells, AWK	
Feb 7	Working with data: relational databases, pandas	
Feb 14, 21	Molecular orbital theory and practice	1,3,5
Feb 28	Electron correlation, density functional theory	4,6
Mar 7	Optimization and molecular properties	11-13
Mar 21, 28	Molecular mechanics and dynamics	2,15
Apr 4	Condensed phases, connections to thermodynamics	14,15
Apr 11, 18	Biomolecular simulations; connections to experiment	
Apr 25, May 2	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 (50%), and projects/presentations (50%). Midway through the semester, each student will chose 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 presentations 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. You may consult with fellow students on homework and on problem sets, but you must personally prepare and understand any written material you hand in. You may *not* consult with fellow students on the final project.