Computational Chemistry
Syllabus for Spring 2023 Term

GENERAL INFORMATION

RUTGERS CATALOG DESCRIPTION

50:160:447 Computational Chemistry (3): Application of the concepts and techniques of modern computational chemistry to physical organic chemistry and biochemistry. Lecture and computer laboratory. **Prerequisites:** 50:160:326 (Instrumental Analysis), 50:160:336 (Organic Chemistry II); and 50:640:221 (Calculus III); or permission of instructor.

AT THE GRADUATE LEVEL

50:160:547 Computational Chemistry (3): Application of the concepts and techniques of modern computational chemistry to physical organic chemistry and biochemistry. Lecture and computer laboratory. **Prerequisites:** No formal prerequisites but students should consult with the instructor and with their research/program advisors to confirm that the course is appropriate for their background and their course of study.

Course Format: Lectures + Computer laboratories

Instructor: **Dr. Guillaume Lamoureux**
Office: Joint Health Sciences Center 216C
Office Hours: By appointment
Email: guillaume.lamoureux@rutgers.edu
Website: http://lamoureuxlab.org/teaching.html

Lectures: Mondays from 6:00 PM to 8:50 PM
Location: BSB-336

Textbooks: The course will require the use of multiple textbooks, available through the Robeson Library (see the Reading Material section below).

COURSE OBJECTIVES

The course presents an introduction to the field of computational chemistry. By the end of the course, students will be expected to understand the main concepts and methods of computational chemistry and how they can be applied to research in organic chemistry and biochemistry. The following topics will be covered: (1) Potential energy surface exploration, (2) Molecular mechanics, (3) Electronic structure calculations, (4) Molecular properties in gas phase and in solution, (5) Molecular dynamics, (6) Structure and dynamics of biomolecules.

COURSE GRADE

The final grade for the course is composed as follows: **30% for the online "lab forms" (10% each), 30% for the lab write-ups (10% each), 30% for the journal club presentation, and 10% for journal club participation**. The minimum passing grade for the course is 60%.

READING MATERIAL

The following textbooks are available for online consultation at the Robeson Library and it is advised that you consult them throughout the course. Specific sections from each textbook will be recommended as the course proceeds.

Textbooks with an emphasis on quantum chemistry:

- **Christopher J. Cramer, *Essentials of Computational Chemistry: Theories and Models*, 2nd Edition (2004).** Covers many topics in detail. Especially good on the topic of density functional theory (DFT). Challenging read if you have no previous exposure to quantum chemistry.
- **Frank Jensen, *Introduction to Computational Chemistry*, 3rd Edition (2017).** Another very complete and detailed source, including more recent developments such as polarizable force fields and dispersion-corrected functionals.
- **Jan H. Jensen, *Molecular Modeling Basics*, 2nd Edition (2010).** Compact and approachable presentation of the main topics. First book to consult whenever it is related to the material of the course.
- **Steven M. Bachrach, Computational Organic Chemistry, 2nd Edition (2014).** Brief presentation of the main methods of computational chemistry, followed by a wealth of applications and case studies.

Textbooks with an emphasis on modelling and simulation:

- **Andrew R. Leach, *Molecular Modelling: Principles and Applications,* 2nd Edition (2001).** Covers a lot of material. Of particular interest for the course are Chapter 4 (empirical force fields), Chapter 5 (energy minimization methods) and Chapter 7 (molecular dynamics methods).
- **Alan Hinchliffe, *Molecular Modelling for Beginners*, 2nd Edition (2008).** A less technical exposition of the essential methods. First half of the textbook presents the principles of molecular mechanics, second half presents the main methods of quantum chemistry.
- **Tamar Schlick, *Molecular Modeling and Simulation: An Interdisciplinary Guide*, 2nd Edition (2010).** Detailed presentation of the techniques of molecular modeling applied to biomolecules (proteins and nucleic acids).

COURSE MATERIAL

All material for the course (except the textbooks listed above) will be posted on Canvas (https://canvas.rutgers.edu). Please consult the website regularly and set your notifications so that you get informed of any updates.

BEFORE EACH LECTURE

Students are expected to do the recommended readings before the lecture and to come prepared with questions and with specific learning objectives. All reading recommendations will be posted on Canvas ahead of time.

BEFORE EACH LAB

The protocols will be made available ahead of time and should be read and understood before the lab starts. These protocols sometimes point to documentation or scientific articles, which should also be looked at before the lab starts. Students are expected to have access to a laptop computer that they can bring in class on the days the laboratories will be performed. (Please contact the instructor as soon as possible if you need another solution to be arranged.) The laptop should have a working wireless connection to the Rutgers University network and a web browser.

ACADEMIC INTEGRITY

Rutgers University takes academic dishonesty very seriously. By enrolling in this course, you assume responsibility for familiarizing yourself with the Academic Integrity Policy and the possible penalties (including suspension and expulsion) for violating the policy. As per the policy, all suspected violations will be reported to the Office of Community Standards. Academic dishonesty includes (but is not limited to): cheating, plagiarism, aiding others in committing a violation or allowing others to use your work, failure to cite sources correctly, fabrication, using another person's ideas or words without attribution, re-using a previous assignment, unauthorized collaboration, sabotaging another student's work. If in doubt, please consult the instructor. Please review the Academic Integrity Policy at http://academicintegrity.rutgers.edu.

STUDENTS WITH DISABILITIES

Rutgers University welcomes students with disabilities into all of the University's educational programs. In order to receive consideration for reasonable accommodations, a student with a disability must contact the appropriate disability services office at the campus where you are officially enrolled, participate in an intake interview, and provide documentation: https://ods.rutgers.edu/students/documentation-guidelines. If the documentation supports your request for reasonable accommodations, your campus's disability services office will provide you with a Letter of Accommodations. Please share this letter with your instructors and discuss the accommodations with them as early in your courses as possible. To begin this process, please complete the registration form at https://webapps.rutgers.edu/student-ods/forms/registration.

LAB FORMS ("PART A")

In part "A" of each lab, students will be required to fill out and submit an online lab form. The lab form is due after the last session of each lab (see Calendar below).

LAB WRITE-UPS ("PART B")

In part "B" of each lab, each student will be assigned a molecule/reaction/property to investigate using the techniques learned in part "A". A one-page write-up <u>about that second part only</u> is to be submitted by the end of the week the lab is performed (see Calendar below).

JOURNAL CLUB

The journal club presentations will be held on **March 27** and **May 1**. If you are not familiar with the format, please read the Wikipedia entry on it (https://en.wikipedia.org/wiki/Journal_club). For the purpose of this course, it will be adapted as following: (1) Each student will be assigned a presentation date and will be given a research article to read and to present in class. (2) All other students will be required to read the article and to submit ahead of time one question related to the significance of the results presented in the article. (3) The instructor will relay those questions to the student presenting, who will have to address them during the presentation. (4) The presentation will be followed by a question period, during which students and instructor will be allowed to ask further questions. The presentation will be evaluated on the delivery of the material and on the discussion of the results. Evaluation will be done both by the instructor and by the students.

CALENDAR OF LECTURES

Please note that this calendar may change as the semester proceeds. The “Assignment” column describes what is expected for each lab session. “Lab forms” are due at the end of the same day and “Lab write-ups” are due Friday of the same week. For the journal club sessions, the questions should be submitted no later than Friday the week before each presentation.

Date		Topics	Assignment
Jan. 23	Lecture	Introduction, Potential energy surfaces	
Jan. 30	Lecture	Molecular mechanics and Quantum mechanics	
Feb. 6	Lecture	Molecular orbital methods	
Feb. 13	Lecture	Molecular orbital methods (cont’d)	
Feb. 20	Lab 1	Conformers of salicylic acid	Form + Write-up
Feb. 27	Lecture	Density functional theory	
Mar. 6	Lecture	Molecular properties	
Mar. 13		SPRING RECESS (no classes)	
Mar. 20	Lab 2	Dehydration of borneol	Form + Write-up
Mar. 27	Journal club	TBA	Presentation/Q&A
Apr. 3	Lecture	Protein and nucleic acid structure, Force fields	
Apr. 10	Lecture	Molecular dynamics	
Apr. 17	Lecture Lab 3	Molecular dynamics (cont’d) Simulation of the barnase-barstar complex	
Apr. 24	Lab 3	Simulation of the barnase-barstar complex (cont’d)	Form + Write-up
May 1	Journal club	TBA	Presentation/Q&A