

Physical Chemistry Laboratory I: Quantum Chemistry

Syllabus for Fall 2020 Term

GENERAL INFORMATION

RUTGERS CATALOG DESCRIPTION

50:160:347-348 Physical Chemistry Laboratory I,II (1,1): Laboratory experiments that illustrate physical chemistry principles, including research-level equipment and simulations on state-of-the-art workstations. Laboratory fee will be applied. **Corequisite for 50:160:347:** 50:160:345. **Corequisite for 50:160:348:** 50:160:346.

Course Format: Online computer laboratories

Instructor: **Dr. Guillaume Lamoureux**

Office: Joint Health Sciences Center 216C

Office Hours: Immediately after the Tuesday lectures

Any other time: By appointment

Email: guillaume.lamoureux@rutgers.edu

Website: <http://lamoureuxlab.org/teaching.html>

Laboratories: Wednesdays from 2:00 PM to 5:00 PM

Location: Online (<https://canvas.rutgers.edu>)

Textbook: There is no textbook for the course. All material will be posted on Canvas (<https://canvas.rutgers.edu>) ahead of time.

COURSE OUTLINE AND GOALS

The course is designed to provide students with a theoretical/computational application of the concepts learned in the Physical Chemistry I lecture. Students will learn how to acquire, analyze, and present theoretical and computational chemistry data. Since this is an upper level laboratory, it is designed to teach students how to perform at the level of a research laboratory. There will be a focus on technical writing, with standards set to those seen in the peer-reviewed scientific literature.

COURSE GRADE

The final grade for the course is composed as follows: **65% for the “lab forms” (5% for each Tutorial and 10% for each Experiment), 30% for the publication-quality report (Experiment #2), and 5% for the peer-reviewing work.** The minimum passing grade for the course is 60%.

EQUIPMENT & SOFTWARE NEEDED FOR THE ONLINE LABS

To perform the online labs, you will be required to use a laptop computer and to have a phone (iOS or Android) with the “Canvas Student” app installed. Since sound and video will be streamed, it is also recommended to have a reliable internet connection. If you are not sure your internet connection (or data plan) is reliable enough, please contact the instructor during the first week of classes. Please note that technical problems (laptop, phone, internet connection, etc.) will not be considered a valid excuse for not attending a lab or for not submitting an assignment.

BEFORE EACH ONLINE 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.

PARTICIPATION TO ONLINE LABS

Online labs will be held on “Zoom”, which you will need to install on your computer. While you will not be asked to turn your camera or your microphone on during the labs, it is expected that you will participate through the “chat” function. However, be aware that you may have to share your screen (and turn your microphone on) if you encounter a technical problem that cannot be resolved without the instructor looking at your work.

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

For each tutorial and experiment, students will be required to fill out and submit an online “lab form”. The lab form is due at the end of each Tutorial, and after the last session of each Experiment (see Calendar below).

EXPERIMENT #2 REPORT

For Experiment #2 (see Calendar below) a publication-quality written report will be due one week after the end of the experiment. To provide you with experience in writing publication-quality technical documents, the reports will be formatted and written using ACS guidelines for the *Journal of the American Chemical Society* (JACS).

PEER REVIEW OF EXPERIMENT #2 REPORTS

To familiarize you with the peer-review process for research publications, reports for Experiment #2 will be anonymously and randomly redistributed within the class, so that each of you can “peer review” the reports written by two of your classmates. When your own report reviews will be returned, you will have to address your classmates’ concerns and make appropriate corrections.

CALENDAR

Please note that this calendar may change as the semester proceeds. The “Assignment” column describes what is expected from each lab session: “Lab form” means that an online lab form is due at the end of the class and “Report” means that a publication-quality report is due before the next class.

Date		Topics	Assignment
Sep. 2		Introduction to the course	
Sep. 9	Tutorial 1	Introduction to Linux and Jupyter notebooks	Lab form
Sep. 16	Tutorial 2	Plotting in R	Lab form
Sep. 23	Tutorial 3	Building and optimizing molecules with GaussView and Gaussian	Lab form
Sep. 30	Tutorial 4	Visualizing molecular orbitals	Lab form
Oct. 7	Tutorial 5	Predicting IR spectra, Energy scans	Lab form
Oct. 14	Experiment #1	Properties of ethylene	Lab form
Oct. 21		Properties of ethylene (cont'd)	
Oct. 28	Experiment #2	Chemical reactivity of silane	Lab form + Report
Nov. 4		Chemical reactivity of silane (cont'd)	
Nov. 11	Experiment #3	HOMO-LUMO gap of hydrocarbons	Lab form
Nov. 18		HOMO-LUMO gap of hydrocarbons (cont'd)	
Nov. 25	NO LAB		
Dec. 2	Experiment #4	Naphthalene versus azulene	Lab form
Dec. 9		Naphthalene versus azulene (cont'd)	