

# Physical Chemistry Laboratory I: Quantum Chemistry

## Syllabus for Fall 2022 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](mailto:guillaume.lamoureux@rutgers.edu)

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

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

Location: BSB-134

**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 expose students to computational applications of the concepts learned in the Physical Chemistry I lecture. Students will learn how to acquire, analyze, and present computational chemistry data. 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: **60% for the “lab forms” (5% for each Tutorial and 10% for each Experiment), 20% for the first report (Experiment #2), and 20% for the second report (Experiment #4).** The minimum passing grade for the course is 60%.

### 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. The “Pre-lab” part of the online lab form should be filled out and submitted before the start of the lab.

### 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 Experiment (see Calendar below).

### PUBLICATION-QUALITY REPORTS

For Experiments #2 and #4 (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 written and formatted using ACS guidelines for the *Journal of the American Chemical Society* (JACS).

## 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>.

## CALENDAR

Please note that this calendar may change as the semester proceeds. The "Assignment" column describes what needs to be turned in for each lab session: "Pre-lab form" means that an online pre-lab form is due before the start of the class, "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. 7	ONLINE	Introduction to the course	
Sep. 14	Tutorial 1	Building and optimizing molecules with GaussView and Gaussian	Lab form
Sep. 21*	Tutorial 2	Introduction to Linux and R	Lab form
Sep. 28	Tutorial 3	Visualizing molecular orbitals	Lab form
Oct. 5	Tutorial 4	Predicting IR spectra, Energy scans	Lab form
Oct. 12	Experiment #1	Properties of ethylene	Pre-lab form**
Oct. 19*		Properties of ethylene (cont'd)	Lab form
Oct. 26	Experiment #2	Chemical reactivity of silane	Pre-lab form**
Nov. 2		Chemical reactivity of silane (cont'd)	Lab form + Report
Nov. 9	Experiment #3	HOMO-LUMO gap of hydrocarbons	Pre-lab form**
Nov. 16*		HOMO-LUMO gap of hydrocarbons (cont'd)	Lab form
Nov. 23	NO LAB		
Nov. 30	Experiment #4	Naphthalene versus azulene	Pre-lab form**
Dec. 7		Naphthalene versus azulene (cont'd)	Lab form + Report

\*\* to be submitted before the class starts