

Physical Chemistry Laboratory I: Quantum Chemistry

Syllabus for Fall 2019 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: Computer laboratories

Instructor: **Dr. Guillaume Lamoureux**

Office: Joint Health Sciences Center 216C

Office Hours: Mondays from 1:00 PM to 1:50 PM (before the lecture)

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: BSB-134

Textbook: There is no textbook for the course. All material will be emailed to you and posted on Sakai (<https://sakai.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 strong 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: **50% for the notebooks (2% for each Tutorial notebook and 10% for each Experiment notebook), 20% for the first report (Experiment #2), 20% for the second report (Experiment #4), and 10% for the peer-reviewing work.** The minimum passing grade for the course is 60%.

PLAGIARISM AND OTHER FORMS OF ACADEMIC DISHONESTY

Please review Rutgers University's Academic Integrity Policy (<http://academicintegrity.rutgers.edu/academic-integrity-policy/>). Any form of unauthorized collaboration, cheating, copying or plagiarism found in this course will be reported and the appropriate sanctions applied. Ignorance of the policy is no excuse and will not result in a reduced sanction.

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>.

JUPYTER ELECTRONIC NOTEBOOKS

Electronic notebooks are due at the end of each tutorial/experiment session (see Calendar below). They should be submitted by email to the instructor in “.ipynb” format before leaving the lab. (Please include the word “PCHEM1” in the subject of your email.) Electronic notebooks are expected to be clear, concise, and rigorous, and to present the results obtained during the laboratory and all the information needed to independently reproduce them.

PUBLICATION-QUALITY REPORTS

For Experiments #2 and #4 (see Calendar below), reports are 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). This will be time consuming and should not be left to the last minute.

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 distributed within the class for you to “peer review” a report written by one of your classmates. When your own reviewed report will be returned, you will have to address your classmate’s 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: “Notebook” means that an electronic notebook 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. 4	Introduction to the course and the online resources	
Sep. 11	Tutorial 1 Introduction to Linux and Jupyter notebooks	Notebook
Sep. 18	Tutorial 2 Plotting in R	Notebook
Sep. 25	Tutorial 3 Building and optimizing molecules with GaussView and Gaussian	Notebook
Oct. 2	Tutorial 4 Visualizing molecular orbitals	Notebook
Oct. 9	Tutorial 5 Predicting IR spectra, Energy scans	Notebook
Oct. 16	Experiment #1 Properties of ethylene	Notebook
Oct. 23	Properties of ethylene (cont'd)	Notebook
Oct. 30	Experiment #2 Chemical reactivity of silane	Notebook
Nov. 6	Chemical reactivity of silane (cont'd)	Notebook + Report
Nov. 13	Experiment #3 HOMO-LUMO gap of hydrocarbons	Notebook
Nov. 20	HOMO-LUMO gap of hydrocarbons (cont'd)	Notebook
Nov. 27	Experiment #4 Naphthalene versus azulene	Notebook
Dec. 4	Naphthalene versus azulene (cont'd)	Notebook + Report
Dec. 11	Due date for Report on Experiment #4	