Physical Chemistry Laboratory I: Quantum Chemistry
Syllabus for Fall 2024 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: **Santanu Malakar**
Office: Chemistry 313
Office Hours: By appointment
Email: santanu.malakar@rutgers.edu

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).

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 according to the standards of peer-reviewed scientific publications.

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), and 40% for the "lab write-ups" (10% for each Experiment)**. 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 ahead 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).

LAB WRITE-UPS

For each experiment (see Calendar below), a publication-quality presentation of the results will be due one week after the end of the experiment. Detailed instructions on how to prepare these writeups will be posted ahead of time. They will typically consist in a table showing the results, accompanied by a caption detailing the calculation procedure.

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 submitted for each lab session. More details on Canvas.

Date	Type	Topics	Assignment
Sep. 4	Introduction	Introduction to the course and Account usage	
Sep. 11	Tutorial 1	Building and optimizing molecules with GaussView and Gaussian, Gas phase vs Solvent Phase calculations	Form
Sep. 18	Tutorial 2	Visualizing MOs and ESPs in GaussView	Form
Sep. 25	Tutorial 3	TS Optimization and Analysis	Form
Oct. 2	Tutorial 4	Optimizing Molecules containing Metals	Form
Oct. 9 Oct. 16	Experiment #1	Properties of ethylene (Assignment Submission deadline Oct 22)	Write-up
Oct. 23 Oct. 30	Experiment #2	Calculation of H-bonding energies and Solvation Energies in gas phase and solvent continuum (Assignment Submission deadline Nov 5)	Write-up
Nov. 6 Nov. 13	Experiment #3	Analyzing Diels-Alder Reactions with DFT (Assignment Submission deadline Nov 19)	Write-up
Nov 20 Nov 27	Experiment #4	Calculating Redox potential of $CoCp^*_2$ vs $FeCp^*_2$ (Assignment Submission deadline Dec 3)	Write-up
Dec 4	Review Week	Review of assignments submitted (if any) – On Zoom	