Physical Chemistry I: Quantum Chemistry
Syllabus for Fall 2020 Term

GENERAL INFORMATION

RUTGERS CATALOG DESCRIPTION

50:160:345-346 Physical Chemistry I,II (3,3): Thermodynamics with chemical applications, kinetics, quantum mechanics, statistical mechanics, transport, and structure. **Prerequisites for 50:160:345:** 50:160:116 & 50:160:126 (Chemical Principles II + Lab), 50:640:221 (Calculus III), 50:750:131-134 (Elements of Physics I & II + Labs). **Prerequisite for 50:160:346:** 50:160:345.

Course Format: Online lectures

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

Lectures: Tuesdays and Thursdays from 9:35 to 10:55
Location: Online (https://canvas.rutgers.edu)

Textbook: **Atkins, De Paula & Keeler, *Atkins' Physical Chemistry*, 11th Edition.**
(The textbook is available for sale at https://universitydistrict.bncollege.com. If you are considering using an earlier edition of the book, please check with the instructor first.)

Review Material: In preparation for the course, please review the following chapters from **Cutnell & Johnson, *Physics*, 10th Edition** (or the equivalent chapters from any other algebra-based Introductory Physics textbook):
- Newton's laws of motion (Chapter 4)
- Rotational motion (Chapters 8 and 9)
- Harmonic motion (Chapter 10)
- Waves (Chapters 16 & 17)
- Electrostatics (Chapters 18 & 19)
- Magnetism (Chapter 21)
- Electromagnetic waves (Chapter 24)

COURSE TOPICS

The course introduces students to the concepts of quantum mechanics and the electronic structure of atoms and molecules. After a review of classical physics, the following topics will be covered: (1) introduction to quantum theory, (2) quantum theory of motion, (3) atomic structure and spectra, (4) molecular structure, (5) rotational, vibrational and electronic spectroscopy, (6) magnetic resonance.

COURSE GRADE

The final grade for the course is composed as follows: **30% for the assignments, 18% for the first midterm exam, 18% for the second midterm exam, and 34% for the final exam**. The minimum passing grade for the course is 60%.

ONLINE COURSE MATERIAL
All material for the course (except the textbook) 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.

EQUIPMENT & SOFTWARE NEEDED FOR THE ONLINE LECTURES AND EXAMS
It is recommended to attend the online lectures using 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 considering using only your phone, or 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 lecture or for not submitting an assignment or an exam.

BEFORE EACH ONLINE LECTURE
A number of pre-recorded mini-lectures will be made available ahead of each lecture. They should be watched before attending the online lecture. Students are also expected to read the appropriate sections of the textbook ahead of time.

PARTICIPATION TO ONLINE LECTURES
Online lectures 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 lectures, it is expected that you will participate through the "chat" function and will remain available for the entire time of the lecture to answer questions or join the discussion.

EXAMINATIONS
The midterm exams will be held on **October 8** and **November 12**. The final exam date is set by the Office of Scheduling and will be announced later during the term. If a student is absent from a midterm exam, he/she must produce a note appropriately signed (e.g., by a doctor or an employer) on letterhead paper. This note must be delivered to the instructor no later than one week after the exam date. If the absence is not valid, the student will receive a mark of zero for the missed exam. If it is valid, the two other exams will be worth 70% of the final grade.

ONLINE EXAMINATIONS
The exams (midterms and final) will be written at home and submitted electronically in PDF format, using a scanning app such as "Notes" (for iOS phones) or "Google Drive" (for Android phones). Students will be responsible for testing the online examination procedure ahead of time, to make sure they can receive and view the exam questions and submit their answers on time. Answers received after the submission deadline will not be accepted.

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.

GRADED ASSIGNMENTS

There will be 3 graded homework assignments during the term. Each assignment will be handed out by the instructor at the end of class and will be due one week later, at the beginning of class. Late assignments will be deduced **10% per day late**. Any assignment handed in more than 4 days late will be given a grade of zero.

PRACTICE PROBLEMS

In addition to the graded assignments, a list of suggested practice problems from the book will be provided with each section. It is the student's responsibility to use these problems to practice in applying the course material.

SOME ADVICE

Note-taking: Take copious notes and keep expanding them as you study and practice the material. Although all overheads will be handed out before the lecture, note-taking is an important exercise in itself. Given the nature of the material (equations and graphs), notes are best taken using either a notebook or loose sheets of paper (numbered, kept in a folder). **Reading/studying:** It is best to read the material on your own first but make sure you eventually meet with your classmates to revise the important concepts and compare your understanding with theirs. The best way to understand something is to try explaining it to somebody else. **Practice problems:** Make the most of the time you spend on each practice problem by asking yourself: What are the concepts or skills being learned? What other similar questions could be asked on the topic? How would the solution/answer change if piece of information "X" in the statement of the problem was changed to "Y"? Could the problem be posed in more general/specific terms?

CALENDAR OF LECTURES

Please note that this calendar may change as the semester proceeds. The chapter numbers refer to the 11th edition of the textbook.

Date	Topics	Reading
Sep. 1	Introduction, Review of classical physics	Review C&J
Sep. 3	Review of classical physics (cont'd)	
Sep. 8	NO LECTURE	
Sep. 10	Review of classical physics (cont'd)	
Sep. 15	The origins of quantum mechanics	7A
Sep. 17	Wavefunctions	7B
Sep. 22	Operators and observables	7C
Sep. 24	Operators and observables (cont'd)	
Sep. 29	The quantum theory of motion	7D & 7E
Oct. 1	The quantum theory of motion (cont'd)	7F
Oct. 6	The quantum theory of motion (cont'd)	
Oct. 8	**Midterm Exam #1 (covers Chapter 7)**	

Oct. 13	Hydrogenic atoms	8A
Oct. 15	Hydrogenic atoms (cont'd)	
Oct. 20	Many-electron atoms	8B
Oct. 22	Atomic spectra	8C
Oct. 27	Valence-bond theory, Molecular orbital theory	9A & 9B
Oct. 29	Molecular orbital theory: diatomic molecules	9C & 9D
Nov. 3	Molecular orbital theory: polyatomic molecules	9E
Nov. 5	Molecular orbital theory: polyatomic molecules (cont'd)	
Nov. 10	Molecular symmetry	10A
Nov. 12	**Midterm Exam #2 (covers Chapters 8 and 9)**	
Nov. 17	General features of molecular spectroscopy	11A
Nov. 19	Rotational and vibrational spectroscopy	11B & 11C
Nov. 24	Rotational and vibrational spectroscopy (cont'd)	11D
Nov. 26	NO LECTURE	
Dec. 1	Electronic spectra, Decay of excited states	11F & 11G
Dec. 3	Electronic spectra, Decay of excited states (cont'd)	
Dec. 8	Magnetic resonance: General principles	12A
Dec. 10	Features of NMR spectra	12B
TBA	**Final Exam (cumulative)**	