Physical Chemistry I: Quantum Chemistry
Syllabus for Fall 2023 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:	Lectures
Instructor:	**Dr. Guillaume Lamoureux**
	Office: Joint Health Sciences Center 216C
	Office Hours: By appointment
	Email: guillaume.lamoureux@rutgers.edu
	Website: http://lamoureuxlab.org/teaching.html
Lectures:	Tuesdays and Thursdays from 9:35 to 10:55
	Location: CNS-213
Textbook:	**Atkins, De Paula & Keeler, *Atkins' Physical Chemistry*, 11th Edition.** (The textbook is available for sale at https://universitydistrict.bncollege.com and for short-term loans at the Robeson Library Reserve. 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*, 12th 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)

TOPICS
The course introduces students to the concepts of quantum mechanics and the electronic structure of atoms and molecules. 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.

COURSE GRADE
The final grade for the course is composed as follows: **18% for the assignments, 21% for the first midterm exam, 21% for the second midterm exam, and 40% for the final exam**. The minimum passing grade for the course is 60%.

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.

BEFORE EACH LECTURE
You are expected to read the appropriate sections of the textbook ahead of time and to have identified the concepts you are not clear about.

EXAMINATIONS
The midterm exams will be held on **October 12** and **November 14**. The final exam date is set by the Office of Scheduling and will be announced later during the term. If you are absent from a midterm exam, you must produce a note appropriately signed (e.g., by a doctor or an employer) on letterhead paper. This note must be delivered no later than one week after the exam date. If the absence is not valid, you will receive a mark of zero for the missed exam. If it is valid, the two other exams will be worth 82% of the final grade.

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 assignments during the term. Each assignment will be due one week after it is handed out. **Late assignments will not be accepted.** Assignments are marked in large part on the clarity and completeness of the reasoning. **Every equation used should be referenced to by its number in the textbook and should be briefly explained in words.** Example: "We use equation (7A.6a), which expresses the energy density of a black body (ρ) as a function of the wavelength of the radiation it emits (λ): (and then the equation)". **Algebraic procedures should be first "called" in words.** Examples: "Solving for λ: (and then the solution)", "Substituting this expression for λ in equation (7A.6a): (and then the equation)". In general, aim to present your solutions in the style of the *Examples* from the textbook.

PRACTICE PROBLEMS
A list of suggested practice problems from the book will be provided with each section. It is your responsibility to use these problems to practice in applying the course material.

SOME ADVICE
Note taking: Note taking during class and when reading the textbook is an important exercise in itself, so take copious notes and keep expanding them as you study and practice the material. **Reading/studying:** 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. When you read the textbook, keep track of any question you have. **Practice problems:** It is very unlikely that you will be successful in this course if you do not do the 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. 5	Introduction, The origins of quantum mechanics	7A
Sep. 7	The origins of quantum mechanics (cont'd)	
Sep. 12	Wavefunctions	7B
Sep. 14	Operators and observables	7C
Sep. 19	Operators and observables (cont'd)	
Sep. 21	The quantum theory of motion	7D
Sep. 26	The quantum theory of motion (cont'd)	7E & 7F
Sep. 28	The quantum theory of motion (cont'd)	
Oct. 3	The quantum theory of motion (cont'd)	
Oct. 5	Hydrogenic atoms	8A
Oct. 10	Exercises in class	
Oct. 12	**Midterm Exam #1 (covers Chapters 7 and 8A)**	
Oct. 17	Many-electron atoms	8B
Oct. 19	Atomic spectra	8C
Oct. 24	Atomic spectra (cont'd)	
Oct. 26	Valence-bond theory	9A
Oct. 31	Molecular orbital theory	9B
Nov. 2	Molecular orbital theory: diatomic molecules	9C
Nov. 7	Molecular orbital theory: diatomic molecules (cont'd)	9D
Nov. 9	Exercises in class	
Nov. 14	**Midterm Exam #2 (covers Chapters 8 and 9)**	
Nov. 16	Molecular symmetry	10A
Nov. 21	General features of molecular spectroscopy	11A
Nov. 23	NO LECTURE	
Nov. 28	Rotational and vibrational spectroscopy	11B & 11C
Nov. 30	Rotational and vibrational spectroscopy (cont'd)	11D
Dec. 5	Electronic spectra, Decay of excited states	11F & 11G
Dec. 7	Electronic spectra, Decay of excited states (cont'd)	
Dec. 12	Exercises in class	
TBA	**Final Exam (cumulative)**	