Physical Chemistry I: Quantum Chemistry
Syllabus for Fall 2018 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 include:** Chemistry prerequisites: 50:160:116, 126. Math pre- or corequisites: 50:640:221, and 50:640:250 or 314. Physics prerequisites: 50:750:131-134 or 50:750:203-206. **Prerequisite for 50:160:346:** 50:160:345.

Course Format: Lectures

Instructor: **Dr. Guillaume Lamoureux**
Office: BSB 422
Office Hours: Tuesdays from 11:00 to 12:00 (after the lecture)
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: 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*, 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: **18% for the assignments, 21% for the first in-class exam, 21% for the second in-class exam, and 40% for the final exam**. The minimum passing grade for the course is 60%.

EXAMINATIONS

The in-class exams will be held on **October 4** and **November 8**. 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 an in-class 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 82% of the final grade.

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.

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 5 days late will be given a grade of zero.

READING MATERIAL AND PRACTICE PROBLEMS

The student is expected to read the appropriate sections of the textbook ahead of time. 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 during the lectures and keep expanding them as you study and practice the material. Although all overheads presented in class will be handed out after 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). Taking notes on electronic devices is not recommended. **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. 4	Introduction, Review of classical physics	Review C&J
Sep. 6	Review of classical physics (cont'd)	
Sep. 11	The origins of quantum mechanics	7A
Sep. 13	Wavefunctions	7B
Sep. 18	Operators and observables	7C
Sep. 20	Operators and observables (cont'd)	
Sep. 25	The quantum theory of motion	7D & 7E
Sep. 27	The quantum theory of motion (cont'd)	7F
Oct. 2	Problems in class	
Oct. 4	**In-class Exam #1 (covers Chapter 7)**	
Oct. 9	Hydrogenic atoms	8A
Oct. 11	Hydrogenic atoms (cont'd)	
Oct. 16	Many-electron atoms	8B
Oct. 18	Atomic spectra	8C
Oct. 23	Valence-bond theory, Molecular orbital theory	9A & 9B
Oct. 25	Molecular orbital theory: diatomic molecules	9C & 9D
Oct. 30	Molecular orbital theory: polyatomic molecules	9E
Nov. 1	Molecular symmetry	10A to 10C
Nov. 6	Problems in class	
Nov. 8	**In-class Exam #2 (covers Chapters 8, 9 and 10)**	
Nov. 13	General features of molecular spectroscopy	11A
Nov. 15	Rotational and vibrational spectroscopy	11B & 11C
Nov. 20	Rotational and vibrational spectroscopy (cont'd)	11D & 11E
Nov. 22	THANKSGIVING (no classes)	
Nov. 27	Electronic spectra	11F
Nov. 29	Decay of excited states	11G
Dec. 4	Magnetic resonance: General principles	12A
Dec. 6	Features of NMR spectra	12B
Dec. 11	Problems in class	
Dec. 13	READING DAY (no classes)	
TBA	**Final Exam (cumulative)**	