Chemistry 346 – Physical Chemistry II – Spring 2022

Syllabus

Day/Time: M & W 10:00am - 11:20am

Location:
Though Jan 31,2022: Remote instruction via Webex (meeting links provided on Canvas)
After Jan. 31, 2022: Smith 240

Instructor: Prof. Jenny Lockard
e-mail: jlockard@newark.rutgers.edu

Office hours: M & W 11:30am-12:30pm

Required Text: *Physical Chemistry*, 11th Edition, Peter Atkins
Recommended Text: *Applied Mathematics for Physical Chemistry*, 2nd Edition, James R. Barrante

Grading: Homework and Quizzes: 20%
2 midterm exams: each 20%
Final exam: 40%

Prerequisite courses:
(21:750:204 GENERAL PHYSICS II or 21:640:235 CALCULUS III) and (21:160:313 INORGANIC CHEMISTRY I)

Course Description:
This course will focus on the theory of quantum mechanics and its implications for understanding atomic and molecular structure and spectroscopies. The course will start by introducing and exploring the tools of quantum mechanics including the Schrodinger equation, operators and wavefunctions. We will first apply these quantum mechanical concepts to simple systems and then, in the second part of the course to atoms and molecules. In the third and final part of the course we will cover various spectroscopy methods as the primary tools used in physical chemistry for observing the effect of energy quantization.

Course goals:

- Master fundamental concepts of quantum mechanics including the understanding and use of Schrodinger equation, operators and wavefunctions
- be able to apply quantum mechanical concepts to
    - simple systems such as particle in a box, harmonic operator and rigid rotor
    - one and multi-electron atoms, to derive atomic orbitals
    - molecules, to molecular orbitals
- Master the fundamental concepts of spectroscopy and the use of different spectroscopy methods for probing the quantized rotational, vibrational, and electronic energy in molecules

Lecture topics / Book Chapter sections (Atkins):

Focus 7 Quantum theory

Topic 7A – The origins of quantum mechanics

- Classical physics review – Newton's laws

- Breakdown of classical mechanics → Energy quantization
- Wave-particle duality

Topic 7B – Wavefunctions

- Schrodinger equation
- normalization and constraints on wavefunctions

Topic 7C – Operators and observables

- Operators
- Expectation values and superposition
- Heisenberg uncertainty principle
- Postulates of Quantum Mechanics

Topic 7D – Translational motion

- Particle in a 1D box
- Particle in a 3D box

Topic 7E – Vibrational motion

- Harmonic oscillator

Topic 7F – Rotational motion

- Rigid Rotor
- Angular momentum

– Midterm Exam – 1

Focus 8 Atomic structure and spectra

Topic 8A Hydrogenic atoms

- Hydrogen atom
- Hydrogen-like atoms
- Atomic orbitals

Topic 8B Many electron atoms

- Electron spin
- Helium atom
- Pauli exclusion principle
- Periodic table
- Aufbau Principle

Topic 8C Atomic spectra

- Angular momentum of many electron atoms
- Atomic term symbols

Focus 9 Molecular structure

- Born Oppenheimer Approximation

Topic 9B – 9E

- Molecular orbital theory
- Homonuclear diatomic molecules
- heteronuclear diatomic molecules
- polyatomic molecules

Focus 10 Molecular symmetry

Topic 10A – 10C

- Symmetry
- Point groups, Character Tables
- Applications of symmetry

– Midterm Exam – 2

Focus 11 Molecular spectroscopy

Topic 11A General features of molecular spectroscopy

- Introduction to spectroscopy
- Selection rules

Topic 11B – Rotational spectroscopy

- Rotational energy levels
- microwave spectroscopy

Topic 11C – 11E Vibrational spectroscopy

- Vibrational spectroscopy of diatomic molecules
- Vibrational spectroscopy of polyatomic molecules
- Raman scattering
- Symmetry and vibrational spectroscopy selection rules

Topic 11F – 11G Electronic spectroscopy

- Electronic absorption and emission
- Electronic spectroscopy of diatomic and polyatomic molecules

Focus 12 Magnetic resonance*

- Nuclear magnetism
- Nuclear Magnetic resonance spectroscopy
- Electron spin resonance spectroscopy

- Final Exam -

*If time permits

Academic Integrity

As an academic community dedicated to the creation, dissemination, and application of knowledge, Rutgers University is committed to fostering an intellectual and ethical environment based on the principles of academic integrity. Academic integrity is essential to the success of the University's educational and research missions, and violations of academic integrity constitute serious offenses against the entire academic community. The entire Academic Integrity Policy can be found here:

http://academicintegrity.rutgers.edu/academic-integrity-policy/

Your health and well-being matter, and Rutgers has put in place a number of resources that are intended to help students through the challenges that might emerge during these times. Information on many of these resources appears below. Please let us know immediately if you are experiencing circumstances that are negatively impacting your academic performance. We also strongly encourage you to contact your academic advisor.

Accommodation and Support

Rutgers University Newark (RU-N) is committed to the creation of an inclusive and safe learning environment for all students. RU-N has identified the following resources to further the mission of access and support:

- *Absences:* All students are responsible for timely notification of their instructor regarding any expected absences. The Division of Student Affairs can provide assistant for absences related to religious observance, emergency or unavoidable conflict (illness, personal or family emergency, etc.) Students should refer to the University's Course Attendance policy (10.2.7), for complete expectations and responsibilities. The office can be contacted at: (973) 353-5063 or deanofstudents@newark.rutgers.edu.

- *Disabilities:* The Office of Disability Services (ODS) is responsible for the determination of appropriate accommodations for students who encounter barriers due to disability. Once a student has completed the ODS process (registration, initial appointment, and submitted documentation) and reasonable accommodations are determined to be necessary and appropriate, a Letter of Accommodation (LOA) will be provided. The LOA must be given to each course instructor by the student and follow up with a discussion. This should be completed as early in the semester as possible as accommodations are not retroactive. More information can be found at ods.rutgers.edu. Contact ODS: (973) 353-5375 or ods@newark.rutgers.edu.

- *Temporary Conditions/Injuries:* The Division of Student Affairs can assist students who are experiencing a temporary condition of injury (broken or sprained limbs, concussions, or recovery from surgery). Students experiencing a temporary condition or injury should submit a request for assistance at: https://temporaryconditions.rutgers.edu.

- *Pregnancy:* The Office of Title IX and ADA Compliance is available to assist students with any concerns or potential accommodations related to pregnancy. Students may contact the office at (973) 353-1906 or TitleIX@newark.rutgers.edu.

- *Gender or Sex-Based Discrimination or Harassment:* The Office of Title IX and ADA Compliance can assist students experiencing any form of gender or sex-based discrimination or harassment, including sexual assault, sexual harassment, relationship violence, or stalking. Students can reports an incident to the office at: (973) 353-1906 or TitleIX@newark.rutgers.edu. Incidents may also be reported by using the following link: tinyurl.com/RUNReportingForm. For more information, students should refer to the University's Student Policy Prohibiting Sexual Harassment, Sexual Violence, Relationship Violence, Stalking and Related Misconduct located at: http://compliance.rutgers.edu/title-ix/about-title-ix/title-ix-policies/.

- *Interpersonal Violence:* The Office for Violence Prevention and Victim Assistance can provide any student with confidential support. The office is a **confidential resource** and does **not** have a reporting obligation to report information to the University's Title IX Coordinator. Students can contact the office at: (973) 353-1918 or run.vpva@rutgers.edu. There is also a confidential, text-based line students can text for support: (973) 339-0734.

- *Crisis and Concerns:* The Campus Awareness Response and Education (CARE) Team works with students in crisis to develop a support plan to address personal situations that might impact academic performance. Students may contact the CARE Team at: http://tinyurl.com/RUNCARE or careteam@rutgers.edu.

- *Stress, Worry, or Concerns about Well-Being:* The Counseling Center has confidential therapists available to support students. To schedule an appointment: counseling@newark.rutgers.edu or (973) 353-5805. If a student is not quite ready to make an appointment with a therapist but is interested in self-help, check out *TAO at Rutgers-Newark* for an easy, web-based approach to self-care and support: https://tinyurl.com/RUN-TAO.

- *Emergencies:* Call 911 or contact Rutgers University Police Department (RUPD) at (973) 353-5111.

Learning Resources:

- *Rutgers Learning Center (tutoring services)*
  (973) 353-5608
  https://sasn.rutgers.edu/student-support/tutoring-academic-support/learning-center

- *Writing Center (tutoring and writing workshops)*
  (973) 353-5847
  nwc@rutgers.edu
  https://sasn.rutgers.edu/student-support/tutoring-academic-support/writing-center