JOHN JAY COLLEGE OF CRIMINAL JUSTICE
The City University of New York
524 West 59th Street, New York, NY, 10019

Syllabus for CHE 302, Section 01, Lab/Rec 1-2
Physical Chemistry II
Quantum Mechanics, Theoretical Spectroscopy,
and Scientific Programming/Data Analysis

Professor's name: Nicholas Petraco

Lecture location: 8.72

Laboratory location: 4.69

Office Contact hours: Thursdays 1:30pm and Open Door Policy

E-mail address: npetraco@gmail.com

Course website: https://npetraco.github.io/CHE302/

Course description:

This is a one-semester seminar course in basic quantum chemistry, theoretical
spectroscopy, materials physical properties and scientific data analysis pertinent to
forensic scientists. It is designed to give a forensic scientist a thorough understanding of
the physical principles behind the spectroscopic/optical methods they use in the lab and
how to analyze the data they obtain. The course is also intended to prepare students for
graduate work in forensic science or chemistry. As such, the course material is intended
to further develop critical thinking and problem solving skills.

Learning outcomes:

By the end of the course students will be able to:

- Solve chemical problems, especially those related to forensic science, using the
  methods of quantum mechanics, classical mechanics and optics. Analyze the
  physicochemical/materials data obtained from different sources using scientific
  computing software R (http://www.r-project.org/), Mathematica and other
  scientific software.
- Identify compounds and various materials commonly encountered in forensic
  science, by spectroscopy and microscopy. Utilize scientific data from literature
  searches of the scientific literature.
- Acquire deep understanding of physical phenomena that lead to the appearance of
  molecular spectra and the formation of images in microscopy.

- Describe various perspectives how physicochemical and materials systems work. Recognize the importance of the knowledge at the interface of physics, chemistry, computing, engineering and forensic science.
- Analyze molecular and atomic spectra. Extract information about chemical compounds from their spectral characteristics.
- Recognize the importance of accuracy and objectivity in collecting physicochemical data, especially with applications to the law.

Science course pre-requisites or co-requisites

Students should have taken PHYS 203/204 (General Physics I and II with Calculus),

CHE 320 (Instrumental Methods I), MAT 241/242 (Calculus I and II) or be enrolled in

CHE 320/CHE 321 (Instrumental Methods II).

Requirements/course policies:

Course announcements and important reminders will be discussed in class and emailed to you. ***As such you must give me email addresses that you check on a regular basis, including your John Jay email***. Home work, labs and exams will be administered through WebAssign. See below for details.

> **Students must check the course website and the e-mail account(s) they gave for this course regularly.**
>
> Students are responsible for all course information, assignments, announcements, and communication that occurs in class, through the course website and your email accounts.

Students must be in possession of a laptop running Windows, Mac OS or Linux for this class. If a student is not in possession of a laptop, one can be borrowed from the school. A tablet or Microsoft surface will not suffice for this course. Students are responsible for being in possession of a laptop installed with the course software (R https://www.r-project.org/ and RStudio https://posit.co/download/rstudio-desktop/) before *each and every* lecture and laboratory session.

Attendance in lecture and laboratory is mandatory. More than three unexcused absences from any of these components will result in an automatic failing grade. Unexcused lateness or early departure will count as ½ an absence, up to 30 minutes. After 30 minutes students will be marked absent.

Unethical/unprofessional conduct which includes cheating will result in a failing grade and referral for additional action. These include copying others' work and sharing work when explicitly forbidden. ***Exams must be taken in person, in class***. **No make up exams will be given without prior instructor approval**. Failure to take a scheduled examination in person, in class without valid and independently supported official

documentation from a medical provider at least 48 hours in advance (unless the emergency is induced by force majeure, subsequent to the 48 hour cutoff, where in valid and independently supported official documentation from a medical provider is still required) will result in a zero grade for that examination.

Americans with Disabilities Act (ADA) Policies:
Students with disabilities will be provided reasonable academic accommodations if determined eligible by the Office of Accessibility Services (OAS). Prior to granting disability accommodations in this course, the instructor must receive written verification of a student's eligibility from the OAS which is located at L66 in the new building (212-237-8031). It is the student's responsibility to initiate contact with the office and to follow the established procedures for having the accommodation notice sent to the instructor in enough time to be effective.

Statement of the College Policy on Plagiarism:
"Plagiarism is the presentation of someone else's ideas, words, or artistic, scientific, or technical work as one's own creation. Using the ideas or work of another is permissible only when the original author is identified. Paraphrasing and summarizing, as well as direct quotations require citations to the original source.

Plagiarism may be intentional or unintentional. Lack of dishonest intent does not necessarily absolve a student of responsibility for plagiarism. It is the student's responsibility to recognize the difference between statements that are common knowledge (which do not require documentation) and restatements of the ideas of others. Paraphrase, summary, and direct quotation are acceptable forms of restatement, as long as the source is cited.

Students who are unsure how and when to provide documentation are advised to consult with their instructors. The Library has free guides designed to help students with problems of documentation."

Policy and Source Material:
http://johnjay.jjay.cuny.edu/files/cunypolicies/JohnJayCollegePolicyofAcademicIntegrity.pdf

Required Resources and Electronic Text:

- Computer:

A laptop running Microsoft Windows, Mac OS or Linux operating systems is required for this course. If a student is not in possession of a laptop, one can be borrowed from the school. A tablet or Microsoft surface will not suffice for this course.

- Physical Chemistry: A Molecular Approach.

D. A. McQuarrie and J. D. Simon

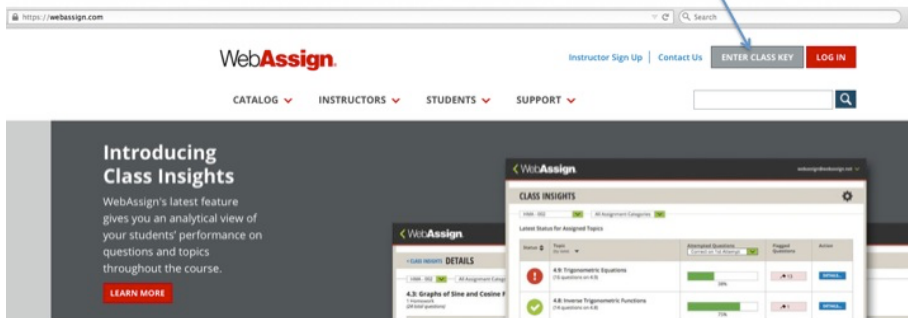- The Assignments/Electronic Text can be purchased on **WebAssign**:

https://webassign.com/

- In order to purchase, got to:

https://www.webassign.net/wa-auth/class-key/enroll

and click on "Enter Class Key" **<u>FOR YOUR SECTION</u>**:

- You should see a place to enter the class key:

  - o Students Registered for **<u>Tuesday</u>** Rec and Lab 10:50am-1:30pm
    - Class Key: **jjay.cuny 8745 4999**
  - o Students Registered for **<u>Thursday</u>** Rec and Lab 10:50am-1:30pm
    - Class Key: **jjay.cuny 4535 3391**

- After entering class key, eventually the website will prompt you to purchase the materials for the class:

- Purchase the **<u>E-textbook and Homework</u>**, which should be **$116.90**

A physical copy of the text is not required, but recommended. It is commonly available at very low cost (~$30 - $50), ISBN-10: 0935702997. John Jay Library does not own a copy unfortunately.

Grading:
<u>Exams</u>
There will be two regular exams and a final (exam III). Regular exams will take place during the lab period to minimize time pressure. The final (exam III) will take place during the scheduled time, finals week. Exam II and the final (exam III) are semi-cumulative in that all exams build on the concepts of the previous exams. Concepts and methods from the earlier parts of the semester will appear on exams during later parts of the semester. That said, reviews before each exam will be thorough, and each exam will emphasize material that has not yet been tested. All exams must be taken in person, in class. Failure to take an exam in person in class without prior instructor approval and/or arrangements will result in an automatic grade of zero for that exam. Each exam (*i.e.* exam I, II and III) will be worth 25% of the total class grade. See course policy above for missed exams.

<u>Workshops/Laboratories</u>
There will be a workshop and/or computational laboratory exercise for each lab period to accompany lecture. Workshops consist of extended guided tutorials and problem solving with R programming and/or use of a methodology in R followed by a short series of graded questions. Laboratories consist of a short pre-lab discussion of R methodology or programming the student should be familiar with, followed by extended scientific case studies with graded questions. The workshops and laboratories train students on standard statistical analysis tasks for the lab sciences and research. They are designed to make the concepts in lecture concrete and use lab relevant datasets as a medium. The R language and RStudio software will be used throughout. The questions consist of a mixture of numerical, graphical and short responses associated with the example datasets. Collectively the laboratory exercises and workshop questions will be worth 15% of the total class grade and are due approximately one week after they have been introduced. Labs up to one week late can be turned in for a 25% penalty. After one week of unexcused lateness, a lab will receive a zero grade.

<u>Home Work Sets</u>
Each week there will be a short home work set consisting of exercises which reenforce and illustrate the material being discussed in the lecture. They are due one week after they have been assigned. Collectively the homework exercises will be worth 10% of the

total class grade. Home works up to one week late can be turned in for a 25% penalty. After one week of unexcused lateness, HW sets will receive a zero grade.

In summary, the grade for this course will be based on two exams (50%), a final (25%), weekly homework sets (10%) and workshop/laboratory exercises (15%). Thus, the lecture portion of this course is worth 75% of the final grade [50%(Exams I, II) + 25%(Exam III-Final) + 10%(HW Sets)] and the laboratory portion of the course is worth 15% of the final grade.

Course lecture/laboratory/exam calendar:

Week/Days	Lecture Topics	Lab/Rec Topics	Notes	HW, Labs and Exam Dates
Aug 29	Course Overview Software Overview			
Sep 3, Sep 5	Classical Waves Math Review	Workshop: Intro to R		Sep 3: HW Set 1 Due
Sep 10, Sep 12	Quantum Theory I	Workshop: A Little R Programming Lab1: Visualizing the Planck Distribution		Sep 10: HW Set 2 Due
Sep 17, Sep 19	Quantum Theory II Postulates of Quantum Mechanics	Workshop: Intro to Mathematica Problem Set, HW/Lab QA		Sep 17: HW Set 3 Due Sep 19: Lab 1 Due
Sep 24, Sep 26	Particle in a Box	Workshop: Numerov Lab 2: PIAB with Numerov		Sep 24: HW Set 4 Due
Oct 1, Oct 3	A Box of Particles	**Exam 1**		Oct 1: HW Set 5 Due *Oct 1: Lab 2 Due **Exam 1, Tues Lab: Oct 1** **Exam 1, Thurs Lab: Oct 3**
Oct 15, Oct 17	Quantum Oscillators	HW QA	No class Oct 15	
Oct 22, Oct 24	Angular Momentum	Lab 3: Harmonic/Anharmonic		*Oct 24: HW Set 6 Due
Oct 29, Oct 31	The Atomic Model	Workshop: Generating Atomic Orbitals Lab 4: Atomic Orbital Visualization and Inferences		Oct 29: HW Set 7 Due Oct 31: Lab 3 Due
Nov 5, Nov 7	Molecular Orbital Theory	**Exam 2**		Nov 5: HW Set 8 Due *Nov 5: Lab 4 Due **Exam 1, Tues Lab: Nov 5** **Exam 1, Thurs Lab: Nov 7**
Nov 12, Nov 14	Vibrational Spectroscopy	Workshop: Huckel MOs Lab 5: Computing and Sketching MOs		Nov 12: HW Set 9 Due
Nov 19, Nov 21	Electronic Spectroscopy Color Theory and Pigments	Workshop: Interferograms and Fourier Transforms Lab 6: What molecule is it?		Nov 19: HW Set 10 Due Nov 21: Lab 5 Due
Nov 26, *Nov 28*	Color Theory and Pigments	HW QA	No class Nov 28	
Dec 3, Dec 5	Intro to Statistical Mechanics	Work Shop: Colorimetry		Dec 3: HW Set 11 Due Dec 5: Lab 6 Due
Dec 10, Dec 12	Catch up/Review	Lab 7: What color is this stuff?	Last week of classes	Dec 10: HW Set 12 Due *Dec 16: Lab 7 Due
**Dec 19		**Exam 3**		**Exam 3, everyone: Dec 19** **8:00am-10:00am, Room 8.72**

*Thursday **December 19**: Exam III (**Final Exam**), 8:00am-10:00am. [Fall 2024 Final Exam Schedule is posted here](#).