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: WP 106

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

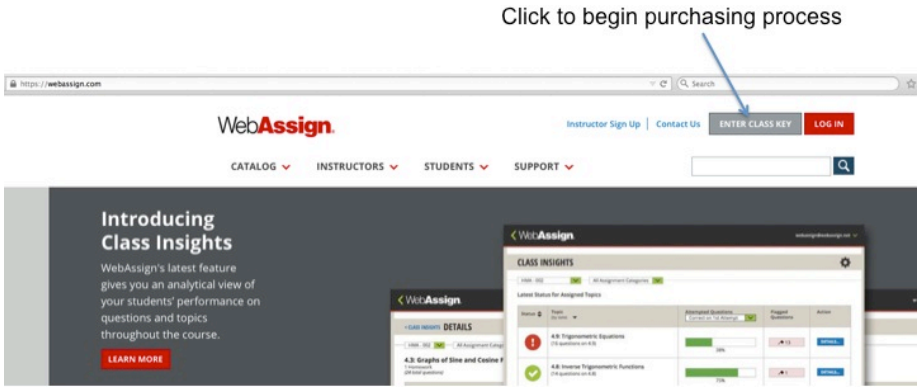
- The Assignments/Electronic Text can be purchased on **WebAssign**:

  https://webassign.com/

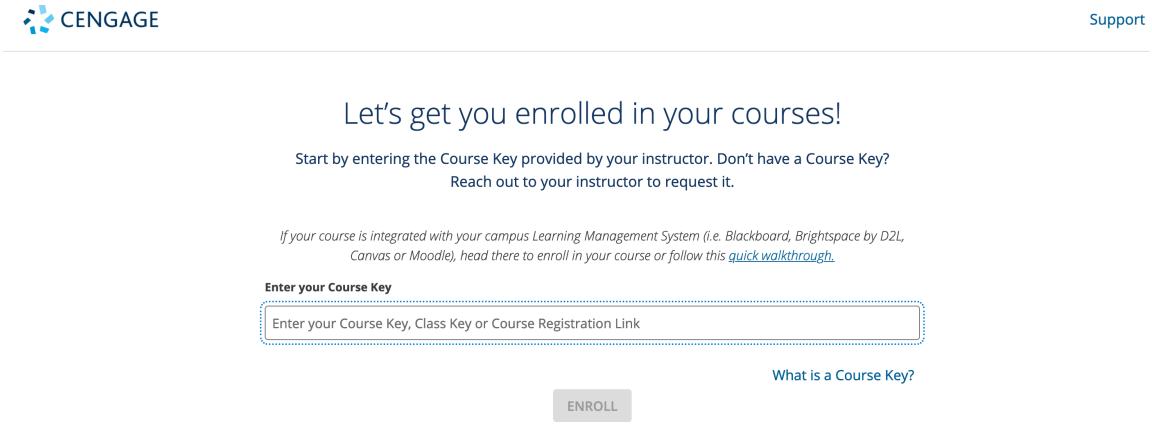
- In order to purchase, got to:

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

  and click on "Enter Class Key" **FOR YOUR SECTION**:

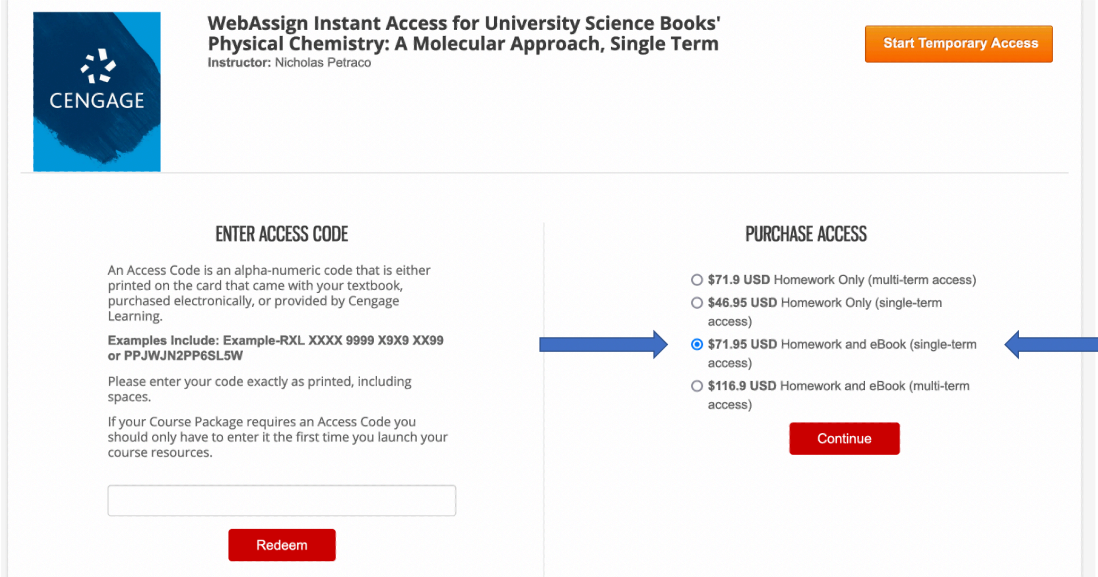


- You should see a place to enter the class key:



  - Students Registered for **Tuesday** Rec/Lab 3:05pm-5:45pm
    - Class Key: **jjay.cuny 3048 0125**
  - Students Registered for **Thursday** Rec/Lab 3:05pm-5:45pm
    - Class Key: **jjay.cuny 1483 5052**

- After logging in/creating-account, eventually the website will prompt you to purchase the materials for the class:



- Purchase the **<u>Single-term E-textbook *AND* the Homework</u>**, which should be **$71.95**

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.

Home Work Sets

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 calendar:

Week/Days	Lecture Topics	Lab/Rec Topics	Notes	HW, Labs and Exam Dates
1/25	Course Overview			
1/30, 2/1	Classical Waves	Workshop: Intro to R Workshop: Intro to Mathematica		
2/6, 2/8	Quantum Theory I	A little scientific programming in R		2/6: HW Set 1 Due
2/13, 2/15	Quantum Theory II	Lab 1: Visualizing the Planck Distribution		2/13: HW Set 2 Due
*2/20	Postulates of Quantum Mechanics	Problem Set	No Class 2/22	2/20: HW Set 3 Due 2/22: Lab 1 Due
2/27, 2/29	Particle in a Box	Workshop: Solving the SE with Numerov		2/27: HW Set 4 Due
3/5, 3/7	Many Particles in a Box: Statistical Mechanics I Intro to the Boltzmann Distribution	**Exam I**		*3/5: HW Set 5 Due **Exam I, Tues Lab: 3/5** **Exam I, Thurs Lab: 3/7**
3/12, 3/14	Oscillation	Lab 2: PIAB with Numerov		3/12: HW Set 6 Due
3/19, 3/21	Angular Momentum	Lab 3: Harmonic/Anharmonic Oscillators with Numerov		3/19: HW Set 7 Due 3/21: Lab 2 Due
3/26, 3/28	Atomic Model	Workshop: Generating Atomic Orbitals Lab 4: Atomic Orbital Vizualization and Inferences		3/26: HW Set 8 Due 3/28: Lab 3 Due
4/2, 4/4	Molecular Orbital Theory	**Exam II**		*4/2: HW Set 9 Due *4/2 Lab 4 Due **Exam II, Tues Lab: 4/2** **Exam II, Thurs Lab: 4/4**
4/9, 4/11	Vibrational Spectroscopy I	Workshop: Huckel MO Theory Lab 5: Computing and Sketching MOs		4/9: HW Set 10 Due
4/16, 4/18	Vibrational Spectroscopy II	Workshop: Interferrograms and Fourier Transforms Lab 6: What Molecule is It?		4/18: Lab 5 Due
*4/23, *4/25			Break, No Class	
*4/30, 5/2	Electronic Spectroscopy	Catch up	No Class 4/30	*5/2: HW Set 11 Due 5/2: Lab 6 Due
5/7, 5/9	Color Theory	Workshop: Colorimetry Lab 7: What Color is this Stuff?		
5/14	Statistical Mechanics II			5/14: HW Set 12 Due *5/14: Lab 7 Due **Exam III, Everyone: May XX XX:XX-XX:XX**

*XX-day **May XX**: **Exam III (Final Exam)**, XX:XXxm-XX:XXxm.