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: 3.78

Laboratory location: 5.67

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

E-mail address: npetraco@gmail.com

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

Americans with Disabilities Act (ADA) Policies – CUNY Accommodations Policy: Students who need an accommodation due to a disability are encouraged to contact the Office of Accessibility Services (OAS) within the first week of class or as soon as possible thereafter. Accommodations can only be approved by the OAS and will be implemented for the student. OAS is located at L66 in the new building, Phone: (212-237-8031), Email: accessibilityservices@jjay.cuny.edu. See CUNY ADA policies for students: Effecting Reasonable Accommodations and Academic Adjustments Procedures Relating to Accommodations and Accessibility for Students (https://www.cuny.edu/about/administration/offices/legal-affairs/policies-procedures/reasonable-accommodations-and-academic-adjustments/)

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 151/152 (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.

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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 (https://www.jjay.cuny.edu/about/governance-senior-leadership/finance-administration/department-information-technology/classroom-lab-support-services/computer-lab-services/laptop-loan-center). A tablet or Microsoft surface will not suffice for this course.

- Text (Online Open Educational Resource):

  Physical Chemistry (LibreTexts) (https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Physical_Chemistry_(LibreTexts))

- Supplementary Text:

  Physical Chemistry: A Molecular Approach.

  D. A. McQuarrie and J. D. Simon

  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.

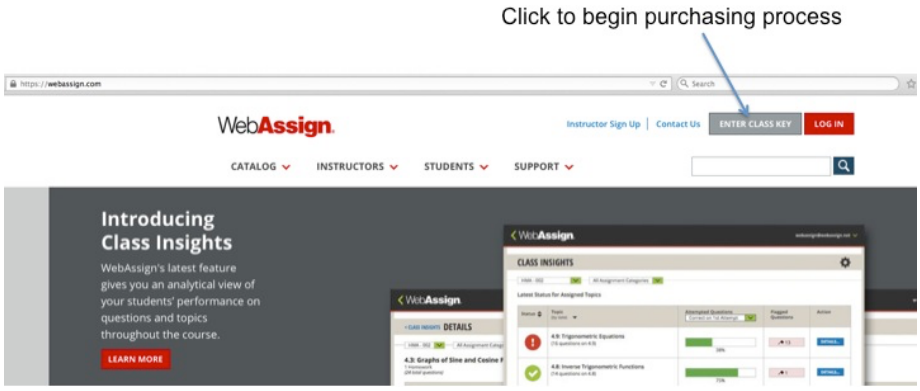
- The Assignments can be purchased on **WebAssign**:

  https://webassign.com/

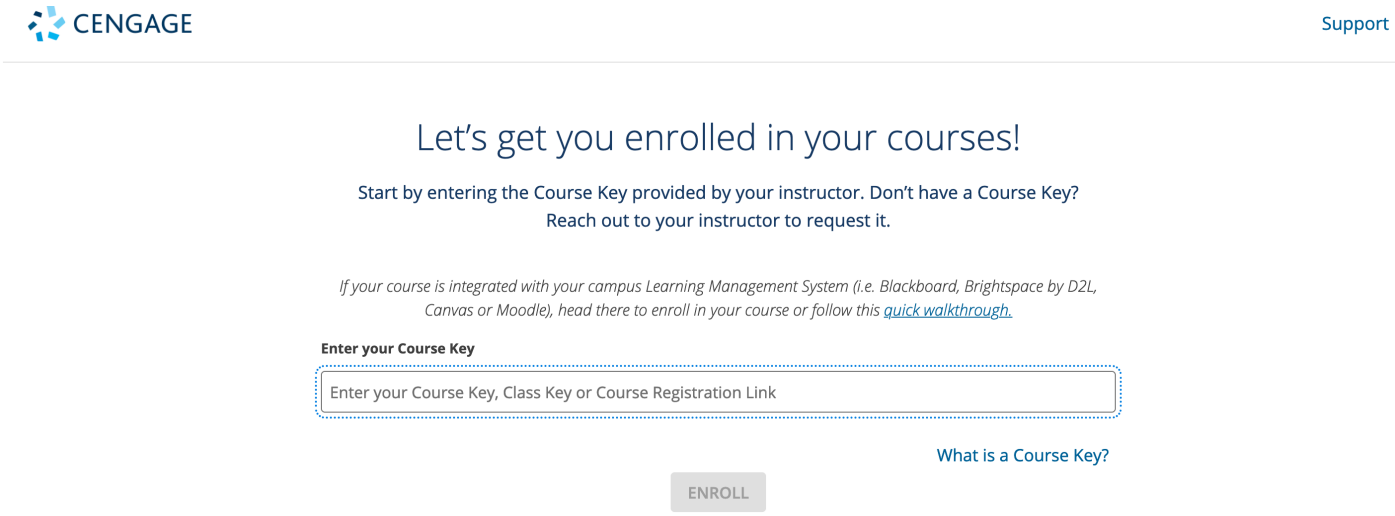
  - In order to purchase, got to:

    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** Laboratory 10:50am-1:30pm
    - Class Key: **jjay.cuny 4417 5989**

  - Students Registered for **Thursday** Laboratory 10:50am-1:30pm
    - Class Key: **jjay.cuny 8225 0751**

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

- Purchase the **Homework Only single-term access**, which should be **$26.95**

Grading:

Exams

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.

Workshops/Laboratories

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/exam calendar:

Days	Lecture Topics	Lab/Rec Topics	Notes/Exams	HW/Labs
Aug 26, Aug 28	Classical Waves	Workshop: Intro to R and Mathematica		
Sep 2, Sep 4	Quantum Theory I	Workshop: A Little R Programming		Sep 2 HW-set 1 due
Sep 9, Sep 11	Quantum Theory II	Lab 1: Visualizing the Planck Distribution		Sep 9 HW-set 2 due
Sep 16, Sep 18	Postulates of Quantum Mechanics	Review and Problem Set		Sep 16 HW-set 3 due Sep 18 Lab 1 due
*Sep 23, Sep 25	Particle in a Box	Thurs Lab/Rec Section **Exam 1**	No class Sep 23 **Exam 1 for Thurs Lab/Rec: Sep 24**	Sep 23 HW-set 4 due
Sep 30, *Oct 2	Particle in a Box	Tues Lab/Rec Section **Exam 1**	**Exam 1 for Tues Lab/Rec: Sep 30** No class Oct 2	
Oct 7, Oct 9	Many Particles in a Box	Numerov workshop		Oct 7 HW-set 5 due
*Oct 14, Oct 16	Oscillation	Lab 2: PIAB with Numerov	No class Oct 14	Oct 16 HW-set 6 due
Oct 21, Oct 23	Angular Momentum	Lab 3: Harmonic/Anharmonic		Oct 21 HW-set 7 due Oct 23 Lab 2 due
Oct 28, Oct 30	Atomic Model	Workshop: Generating Atomic Orbitals Lab 4: Atomic Orbital Visualization and Inferences		Oct 28 HW-set 8 due Oct 30 Lab 3 due
Nov 4, Nov 6	Review and Molecular Orbital Theory	**Exam 2**	**Exam 2 for Tues Lab/Rec: Nov 4** **Exam 2 for Thurs Lab/Rec: Nov 6**	Nov 4 HW-set 9 due Nov 6 Lab 4 due
Nov 11, Nov 13	Vibrational Spectroscopy I	Workshop: Huckel MOs Lab 5: Computing and Sketching MOs		Nov 11 HW-set 10 due
Nov 18, Nov 20	Vibrational Spectroscopy II	Workshop: Interferograms and Fourier Transforms Lab 6: What molecule is it?		Nov 18 Lab 5 due
Nov 25, *Nov 27	Electronic Spectroscopy			Nov 25 HW-set 11 due
Dec 2, Dec 4	Color Theory	Work Shop: Colorimetry Lab 7: What color is this stuff?		Dec 4 Lab 6 due
Dec 9, Dec 11	Statistical Mechanics and Weights of Evidence	Review		Dec 9 HW-set 12 due Dec 11 Lab 7 due
Dec XX			**Final/Exam 3 12/XX** **XX:XXxm-XX:XXxm**	

*XXXXday **December XX**: **Final Exam** (**Exam 3**), XX:00xm-XX:00xm (LINK)