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: 6.67

Laboratory location: 6.61

Contact hours: Fridays 12:00 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, optics, materials 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 optical and electron 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.

- Collect and 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.

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) and be enrolled in CHE 321 (Instrumental Methods II).

Requirements / course policies

Unethical/unprofessional conduct which includes cheating will result in a failing grade and referral for additional action. *Attendance in lecture laboratory and recitation is mandatory*. More than five 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 you will be marked absent.

Required Electronic Text and Resources:

Physical Chemistry: A Molecular Approach.

D. A. McQuarrie and J. D. Simon

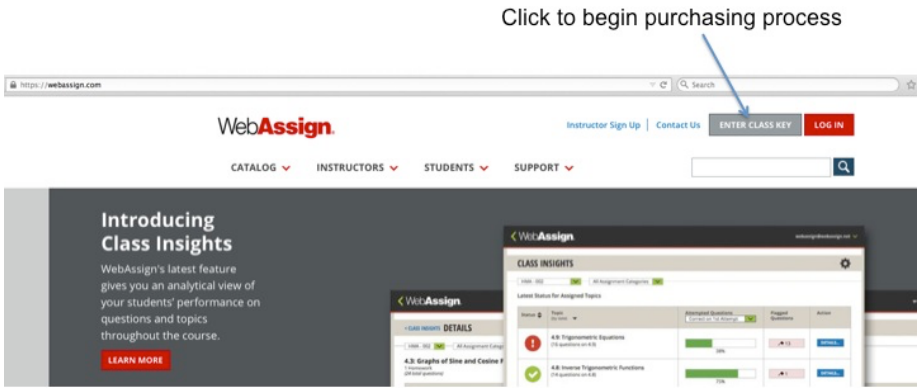
- The Assignments/Electronic Text can be purchased on **WebAssign**:

  https://webassign.com/

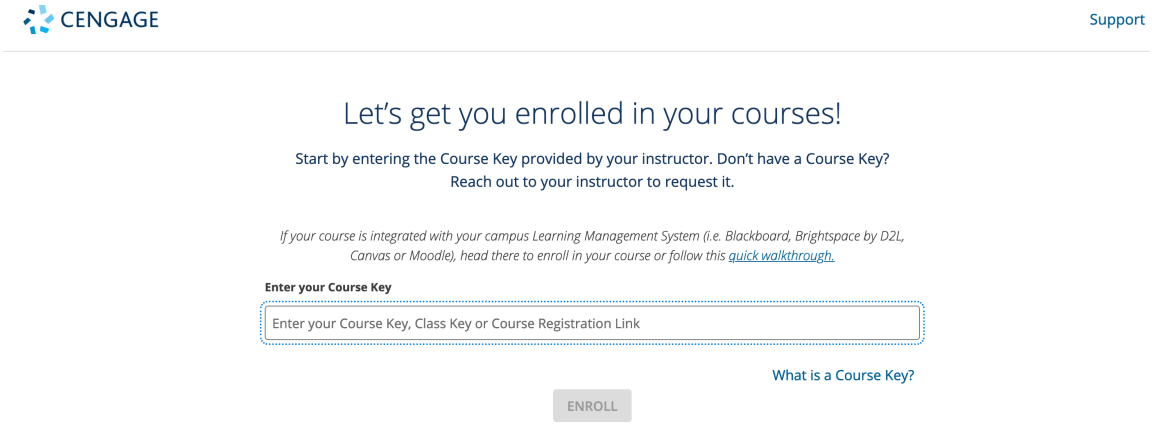
- In order to purchase, got to:

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

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

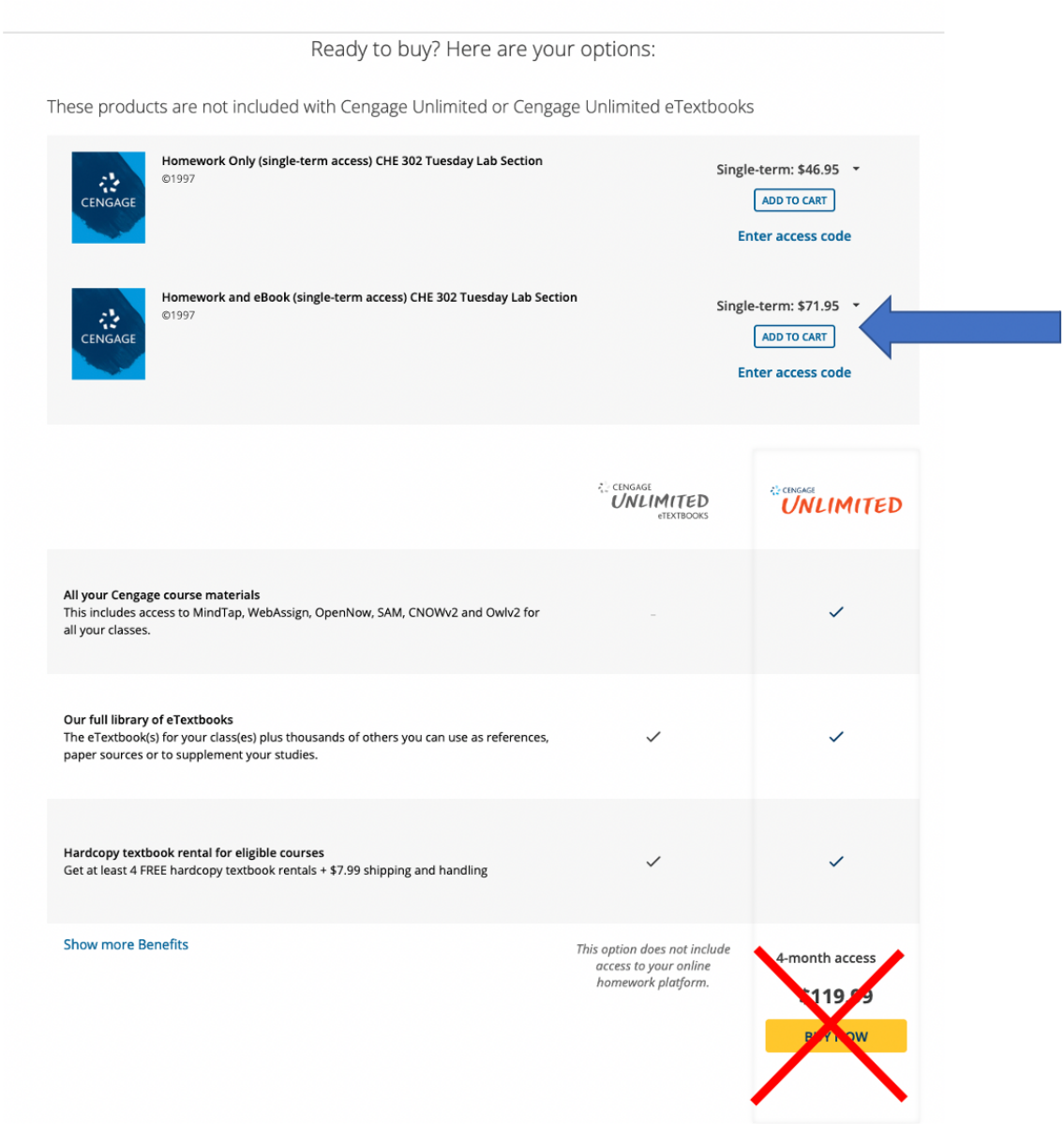


- You should see a place to enter the class key:



  - Students Registered for **Tuesday** Rec/Lab 3:05pm-5:45pm
    - Class Key: **jjay.cuny 3194 5953**
  - Students Registered for **Thursday** Rec/Lab 3:05pm-5:45pm
    - Class Key: **jjay.cuny 2237 9032**

- 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:

The grades for this course are based on home works (10%), two exams (50%), a final

(25%) and laboratory exercises (15%).

Course lecture/laboratory calendar:

- August 26: Syllabus Review. Course Overview.
- August 31, September 2: Syllabus Review. Course Overview. Classical Waves
    - Algebra and calculus refresher/Basic R and Mathematica tutorial.
- September 9: Quantum Theory I.
    - Workshop: Introduction to scientific computing, R and RStudio
    - Lab 1: R on your own, the Planck/Blackbody curve
- September 14: Quantum Theory II.
    - Workshop: Introduction to scientific computing, R and RStudio
    - Lab 1: R on your own, the Planck/Blackbody curve
- September 21, 23: Postulates of Quantum Mechanics. Probability and Statistics Refresher.
    - Intro to the Numerov Programs for Solving the Schrödinger Equation
- September 28, 30: Getting used to the Schrödinger Equation: Particle in a box.
    - Review
    - Lab 2: Particle In a Box Numerov Problems
- October 5, 7: Harmonic/Anharmonic Oscillator.
    - **Exam I** in Lab Section
- October 12, 14: Angular Momentum, Particle on a Sphere.
    - Lab 3: Harmonic and Anharmonic Numerov Problems
- October 19, 21: Atomic Orbitals: The detailed hydrogenic atom. Review.
    - Intro to Numerov for Radial Wave Functions. Sample plotting atomic orbitals.
- October 26, 28: Molecular orbitals, Hückel Model.
    - Lab 4: You solve the hydrogen-like Schrödinger Equation
- November 2, 4: Connections to electronic spectroscopies, UV/Vis.
    - **Exam II** in Lab Section
- November 9, 11: Molecular geometries, normal mode analysis.
    - Intro to Matrix Mechanics on a Computer/Computational Hückel Method

- November 16, 18:
    - Lab 4: Hückel on your own
- November 23: Fourier Transforms Infrared (Vibrational) Spectroscopy.
- November 30, December 2: Fourier Transforms Infrared (Vibrational) Spectroscopy.
    - Intro to Discrete Fourier Transforms in R
- December 7, 9: Light: Color and Filters.
    - Lab 5: From the interferrogram: What's the unknown molecule?
    - Late Assignment Catch-up

*Thursday **December 16**: **Exam III (Final Exam)**, 10:30am-12:30pm.

College wide policies for undergraduate courses *(*see the *Undergraduate Bulletin*, Chapter IV Academic Standards)

A. **Incomplete Grade Policy**

B. **Extra Work During the Semester**

C. **Americans with Disabilities Act (ADA) Policies**

"Qualified 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."

Source: *Reasonable Accommodations: A Faculty Guide to Teaching College Students with Disabilities*, 4th ed., City University of New York, p.3. (http://www.jjay.cuny.edu/studentlife/Reasonable_Accommodations.pdf)

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. *(John Jay College of Criminal Justice Undergraduate Bulletin,* http://www.jjay.cuny.edu/academics/654.php , see Chapter IV Academic Standards)