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

Syllabus for CHE 302, All Sections
Physical Chemistry
Quantum Mechanics, Theoretical Spectroscopy and Scientific Programming

Professor's name: Nicholas Petraco

Office location: 5.64 New Building

Contact hours: Fridays's 11:00 and Open Door Policy

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Course description:

This is a one semester seminar course in basic quantum chemistry, theoretical spectroscopy and scientific data analysis. 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 chemistry or forensic science. 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 approach of quantum mechanics and classical mechanics and optics. Analyze the physicochemical/materials data obtained from different sources using scientific computing software R and Mathematica.
- 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 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.

Texts

- **Required**:
    1. Physical Chemistry: A Molecular Approach.
        i. D. A. McQuarrie and J. D. Simon
        ii. ISBN-10: 0935702997
            1. Text is ordered and should be available in the bookstore
            2. John Jay Library does not own a copy unfortunately
            3. www: http://www.amazon.com/Physical-Chemistry-Molecular-Donald-McQuarrie/dp/0935702997/ref=pd_bbs_sr_1?ie=UTF8&s=books&qid=1232842813&sr=8-1

Grading

- The grades for this course are based on two exams (50%) and two extended problem sets/ programming projects (50%). Short problem sets will also be given out during recitations to reinforce the lecture material.

Course calendar

- January 29,31: Classical Waves. Basic R input/output and plotting.
- February 5,7: Basic Quantum Theory.
- February 14: Schrodinger equation and simple potentials. Numerical solutions in R.
- February 19,21: Particle in a Box, Harmonic oscillator. Practice R problem set due.
- February 26,28: Harmonic oscillator (con't), anharmonic oscillator.

Connections to vibrational spectroscopy.

- March 5,7: Angular momentum, particle on a ring.
- March 12,14: Orbitals: The detailed hydrogenic atom system. Problem set due.
- March 19,21: Molecular orbital theory. Review.
- April 4: In class exam 1.
- April 9,11: The Huckel model. Connections to electronic excitation spectroscopies.
- April 16, 18: Anharmonic oscillator, molecular geometries, molecular symmetry.
- April 23,25: Fourier Transform, IR spectroscopy.
- April 30, May 2: Raman Spectroscopy, UV/Vis spectroscopy. Problem set 2 due.
- May 7,9: Electron Microscopy. Beginning X-ray spectroscopy.
- May 14,16: Intro to Statistical Mechanics and Review.

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**

Boilerplate: "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)

Plagiarism detection software - the College subscribes to **Turnitin.com** and Blackboard has a similar module called **SafeAssign.** If you will be using any plagiarism detection software in your course, you must state it on the syllabus.