CHEM356: Physical Chemistry II - Spectroscopy
Syllabus Spring 2019

Instructor: Dr. Mateusz Marianski
Room#: HN-1321B
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Lecture: Tue, 2.10-3.25 pm & Fri 2.10-3.25 pm, **C103**
Office hours: Thu, 4-6 pm, **HN-1312B Office**

Text: Physical Chemistry
Thomas Engel, Phillip Reid
3^{rd} edition, Pearson

Supplemental reading: Physical Chemistry: Molecular Approach
John McQuarrie, John Simons
3^{rd} edition,

Slides and notes: Some lectures will be accompanied with slides posted on Blackboard

Course Objectives and Learning Goals

Students in this course will learn basic principles of quantum mechanics. In details, the course is aimed to equip students with understanding of:

- The difference between classical and quantum treatment of matter
- Fundamentals of particle in a box, rigid rotator and harmonic oscillator.
- The solution for hydrogen and hydrogen-line atoms
- Treatment of many-electron atoms and molecules
- Theoretical foundation for spectroscopic methods
- Elements of computational chemistry

Upon completion of this course, students should have a solid understanding of the basic principles of quantum mechanics, theoretical foundation of spectroscopy and computational chemistry. Students should be able to apply the knowledge in future studies and in career in science or related fields. Moreover, students should have enhanced ability to use mathematics to address complex chemical and physical problems, as well as enhanced analytical reasoning and problem-solving skills.

Prerequisites

Participation in the course requires understanding of variety of mathematical tools, namely linear algebra and differential calculus.

Grading and Exams

The lecture is divided into 3 sections. Two problem sets accompany each section. Each problem set is worth 25 pts, the due dates are listed in the table. Each section will be concluded with an 75-minutes exam (100 pts).
Only a letter-sized sheet of notes is allowed for the exam. Bring calculators - mobile-phone substitutes are not allowed.
Students are expected to take exams at the scheduled time with the entire class. There are no makeups for exams (Department policy)
In-class project worth 50 pts will be assigned in the third part of the semester individually.
The grade will be calculated on the basis of a percentage of total points (500 pts). The projected grade lines are:

A : 100.0% - 90.0%
B : 89.8% - 80.0%
C : 79.8% - 70.0%
D : 69.8% - 60.0%
F : 59.8% - 0.0%

HC statements:

Academic Integrity Statement: "Hunter College regards acts of academic dishonesty (e.g., plagiarism, cheating on examinations, obtaining unfair advantage, and falsification of records and official documents) as serious offenses against the values of intellectual honesty. The College is committed to enforcing the CUNY Policy on Academic Integrity and will pursue cases of academic dishonesty according to the Hunter College Academic Integrity Procedures."
Cheating will be punished as severely as allowed under University guidelines.

ADA Statement: "In compliance with the ADA and with Section 504 of the Rehabilitation Act, Hunter College is committed to ensuring educational access and accommodations for all its registered students. Hunter College's students with disabilities and medical conditions are encouraged to register with the Office of AccessABILITY for assistance and accommodation. For information and appointment contact the Office of AccessABILITY located in Room E1214 or call (212) 772-4857 /or VRS (646) 755-3129."

Hunter College Policy on Sexual Misconduct: "In compliance with the CUNY Policy on Sexual Misconduct, Hunter College reaffirms the prohibition of any sexual misconduct, which includes sexual violence, sexual harassment, and gender-based harassment retaliation against students, employees, or visitors, as well as certain intimate relationships. Students who have experienced any form of sexual violence on or off campus (including CUNY-sponsored trips and events) are entitled to the rights outlined in the Bill of Rights for Hunter College.

a. Sexual Violence: Students are strongly encouraged to immediately report the incident by calling 911, contacting NYPD Special Victims Division Hotline (646-610-7272) or their local police precinct, or contacting the College's Public Safety Office (212-772-4444).

b. All Other Forms of Sexual Misconduct: Students are also encouraged to contact the College's Title IX Campus Coordinator, Dean John Rose (jtrose@hunter.cuny.edu or 212-650-3262) or Colleen Barry (colleen.barry@hunter.cuny.edu or 212-772-4534) and seek complimentary services through the Counseling and Wellness Services Office, Hunter East 1123. CUNY Policy on Sexual Misconduct Link: http://www.cuny.edu/about/administration/offices/la/Policy-on-Sexual-Misconduct-12-1-14-with-links.pdf"

Tentative Schedule

Table 1: The list of lectures titles, and respective chaptes in the book. The due dates for homework are shown in bold.

#	Class/HW due	Day	Lecture	Chapters
L01	01-25-19	F	From Classical to Quantum Mechanics I	CH 12
L02	01-29-19	T	From Classical to Quantum Mechanics II	CH 12
L03	02-01-19	F	Classical wave and Schrödinger Equation	CH 13
L04	02-05-19	T	The Schrödinger Equation	CH 13
L05	02-08-19	F	The Quantum Mechanical Postulates	CH 14
B	02-12-19	T	No Class	
L06	02-15-19	F	Particle in a Box I	CH 15
L07	**02-19-19**	T	Particle in a Box II	CH 15-16
L08	02-22-19	F	Particle in a Box III	CH 16-17
L09	02-26-19	T	Quantum Rigid Rotator and Harmonic Oscillator I	CH 18
L10	03-01-19	F	Quantum Rigid Rotator and Harmonic Oscillator II	CH 18
L11	03-05-19	T	Physical Basis of Vibrational and Rotational Spectroscopy I	CH 19
L12	03-08-19	F	Physical Basis of Vibrational and Rotational Spectroscopy II	CH 19
E01	**03-12-19**	T	Exam I	
L13	03-15-19	F	The single-electron atom (a.k.a. Hydrogen) I	CH 20
L14	03-19-19	T	The single-electron atom - Atomic Orbitals II	CH 20
L15	03-22-19	F	Many-electron atom - Hellium atom	CH 21
L16	03-26-19	T	Many-electron atom - Variational and perturbation methods	CH 21
L17	**03-29-19**	F	Quantum States for Many-Electron atoms	CH 22
L18	04-02-19	T	Diatomic Molecules and Molecular Orbitials I	CH 23
L19	04-05-19	F	Diatomic Molecules and Molecular Orbitials II	CH 23
E02	**04-09-19**	T	Exam II	
L20	04-12-19	F	Polyatomic Molecules I - Hybrid Orbitals	CH 24
L21	04-16-19	T	Polyatomic Molecules II - The Hückel Model	CH 24
B	04-19-19	F	No Class	
B	04-23-19	T	No Class	
B	04-26-19	F	No Class	
L22	04-30-19	T	Basis of Electronic Spectroscopy	CH 25
L23	05-03-19	F	Energy-transfer Spectroscopy	CH 25
L24	**05-07-19**	T	Computational Chemistry - basis sets	CH 26
L25	05-10-19	F	Computational Chemistry - wavefunction methods	CH 26
L26	05-14-19	T	Computational Chemistry - density-functional theory	CH 26
E03	**05-17-19**	F	Exam III	