CHEM356: Physical Chemistry II - Spectroscopy
Syllabus Spring 202

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

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

Slides and notes: Some lectures will be accompanied with slides posted on Blackboard.
Homeworks will be posted at `marianski-lab.github.io/courses.html`

Course Description

The course will introduce students to fundamentals of quantum mechanics and spectroscopy. During the scope of the course, we will discuss several solvable problems in quantum chemistry and apply them to uderstand basics of molecularspetroscopy. Next, multielectron atoms and molecules will be introduced. The derivation of atomic and molecular terms will be shown. Finally, we will discuss elements of computational chemistry as a scientific tool.

Learning Outcomes

By the end of the semestrer, students will be able to :

- explain the difference between classical and quantum treatment of matter,
- discuss solvable problems of quantum mechanics: a particle in a box, rigid rotator and harmonic oscillator,
- analyze the solution of the schoedinger equation for hydrogen and hydrogen-line atoms,
- identify and write respective terms for the hamiltonian of multi-electon systems,
- assign atomic and molecular terms,
- evaluate the theoretical models used in research papers.

Furhermore, upon completion of this course, students should have a solid understanding of fundamentals of quantum mechanics and basic knowledge of computational chemistry and spectroscopy which they will be able in future study and/or in career in science or related fields. Moreover, the course aims at enhancing the students' ability to apply mathematics to address complex chemical and physical problems, as well as enhanced analytical reasoning and problem-solving skills.

Prerequisites

CHEM 249 and MATH 150 (soon to be changed!) and PHYS 121 all with a grade of C or better.

In addition to the offical prerequisites, successful participations in the course requires understanding of variety of mathematical tools, namely logarithms, differential calculus and linear algebra. Review of these topics is up to a student own interest.

Grading and Exams

Homeworks The lecture is divided into 4 sections . One problem sets, worth 20 pts, accompanies each section. The due dates are listed in the table.

Exams Each section will be concluded with a 75-minute exam (30 pts). One letter-sized sheet of notes is allowed for the exam. Please 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)

Project The final 50 points will be graded from a presentation of a research paper in computational discussion and participation in a discussion following each presentation.

The grade will be calculated on the basis of a percentage of total points (500 pts). The projected grade lines are:

A : 90.2% - 100.0% / 225 - 250 pts.
B : 80.2% - 90.0% / 200 - 224 pts.
C : 70.2% - 80.0% / 175 - 199 pts.
D : 60.2% - 70.0% / 150 - 175 pts.
F : 0.0 % - 60.0% / $<$ 150 pts.

The full grades are divided into X+, X and X- using >x7.4%, x2.6% - x7.4% and <x2.4% ranges.

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."

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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 and respective chapters in McQuarrie. The homework due dates are shown in bold.

#	Class/HW due	Day	Lecture	Chapters
L01	01-28-19	T	From Classical to Quantum Mechanics I	CH 1
L02	01-31-19	F	From Classical to Quantum Mechanics II	CH 1
L03	02-04-19	T	Classical wave equation	CH 2
L04	02-07-19	F	The Schrödinger Equation	CH 3
L05	02-11-19	T	Particle in the 1D and 2D Box	CH 3
L06	02-14-19	F	Postulates of Quantum Mechanics I	CH 4
L07	02-18-19	T	Postulates of Quantum Mechanics II	CH 4
E01	02-21-19	F	Exam I	CH 1-4
L08	**02-25-19**	T	The Harmonic Oscillator	CH 5
L09	02-28-19	F	The Rigid Rotator I	CH 5
L10	03-03-19	T	The Rigid Rotator II	CH 5
L11	03-06-19	F	The single-electron atom I - Hydrogen atom	CH 6
L12	03-10-19	T	The single-electron atom II - Atomic Orbitals	CH 6
E02	03-13-19	F	Exam II	CH 5-6
L13	**03-17-19**	T	Introduction to Approximation Methods	CH 7
L14	03-20-19	F	Multielectron Atoms	CH 8
L15	03-24-19	T	Multielectron Atoms - Terms	CH 8
L16	03-27-19	F	Diatomic Molecules I	CH 9
L17	04-31-19	T	Diatomic Molecules II	CH 9
E03	04-03-19	F	Exam III	CH 6-9
B	04-07-19	T	Wednesday Schedule	
B	04-10-19	F	No Class	
B	04-14-19	T	No Class	
L18	**04-17-19**	F	Polyatomic Molecules I - Hybrid Orbitals	CH 10
L19	04-21-19	T	Polyatomic Molecules II - The Hückel Model	CH 10
L20	04-24-19	F	Molecular Simulations - Introduction	assign
L21	04-28-19	T	Comutational Chemistry - Introduction	assign
L22	05-01-19	F	Molecular Spectroscopy I	CH 13
L23	05-05-19	T	Molecular Spectroscopy II	CH 13
L24	05-08-19	F	Computational Chemistry - Presentations I	assign
L25	**05-12-19**	T	Computational Chemistry - Presentations II	assign
B	05-15-19	F	Reading Day	
FIN	05-19-19	T	Final Exam (11.30 - 1.30 pm)	Comp and Spectro