Fall 2020

CHEM 658-101: Advanced Physical Chemistry

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NJIT New Jersey Institute of Technology

THE COLLEGE OF SCIENCE AND LIBERAL ARTS

THE DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE

Chemistry:
Fall 2020 Course Syllabus

NJIT Academic Integrity Code: All Students should be aware that the Department of Chemistry & Environmental Science (CES) takes the University Code on Academic Integrity at NJIT very seriously and enforces it strictly. This means that there must not be any forms of plagiarism, i.e., copying of homework, class projects, or lab assignments, or any form of cheating in quizzes and exams. Under the University Code on Academic Integrity, students are obligated to report any such activities to the Instructor.

COURSE INFORMATION

Course Description: Principles and applications of quantum chemistry; the wave equation, its properties and mathematics; the Schrodinger equation and wave functions; the harmonic oscillator; atomic theory, structure, and properties; simple molecules, LCAO and valence bond theories; time dependence, and introduction to electronic and vibration-rotation spectroscopy.

Number of Credits: 3

Prerequisites:

CHEM336: MATH 222 and CHEM 126 with a grade of C or better
CHEM658: one year of undergraduate physical chemistry

Course-Section and Instructors

Course-Section	Instructor
CHEM 336-101, R 6pm – 8:50 pm	Farnaz A. Shakib
CHEM 658-101, R 6pm – 8:50 pm	Farnaz A. Shakib

Office Hours: Tuesdays 6 pm – 8:50 pm

Required Textbook:

Title	Quantum Chemistry
Author	Donald A. McQuarrie
Edition	Second
Publisher	University Science Books
ISBN #	978-1-891389-50-4

University-wide Withdrawal Date: The last day to withdraw with a **W** is Monday, November 09, 2020. It will be strictly enforced.

Learning Outcomes: At the end of the course, the student will be able to

- Describe the concept of energy quantization and wave-particle duality of light and matter
- Describe the differences between classical and quantum mechanics
- Construct the Schrödinger equation for simple systems
- Normalize a wavefunction and calculate the probability density of a system in a region
- Construct quantum chemical operators and determine expectation values of observables
- Describe the solution of the Schrödinger equation for a free motion in one dimension and confined motion in one and two dimensions and calculate their properties.
- Use the separation of variables technique
- Describe the solution of the Schrödinger equation for a harmonic oscillator and calculate it's properties.
- Describe the solutions of the Schrödinger equation for hydrogenic atoms and their properties: quantum numbers, orbital energies, classification in shells
- Construct a wavefunction for a many-electron atom using the orbital approximation
- Interpret atomic spectra of hydrogenic atoms and complex atoms using selection rules and assign term symbols to electronic states of atoms
- Explain the concept of hybridization and molecular orbital theory
- Assign ground state electron configurations to homo- and heteronuclear diatomic molecules
- Use the Hückel approximation to calculate the π-electron binding energy in aromatic molecules.
- Explain the fundamental concepts of absorption and emission spectra
- Calculate moments of inertia of simple molecules and classify them as rotors
- Interpret IR-spectra of diatomic and polyatomic molecules using selection rules
- Interpret electronic spectra of molecules using selection rules

Canvas: There is a course Canvas site that will include significant resources and updates of importance to this course, both for the lecture and laboratory portions. Please check it frequently, and also make sure to check or forward your NJIT email in order to receive important announcements. Furthermore, all the office hours and discussions will be conducted through Canvas.

POLICIES

All CES students must familiarize themselves with, and adhere to, all official university-wide student policies. CES takes these policies very seriously and enforces them strictly.

Grading Policy: The final grade in this course will be determined as follows:

Homework	20
Class Participation Solving problems in class, active role in asking and answering questions, and lab work	20
Midterm Exam I	20
Midterm Exam II	20
Final Exam	20

Your final letter grade in this course will be based on the following tentative curve:

A	88-100	**C**	60-64.5
B+	78-87.9	**D**	55-59.9
B	70-77.9	**F**	< 55
C+	65-69.9		

Attendance Policy: Attendance at all classes is not mandatory but extremely encouraged due to the nature of the topic which cannot be simply learnt through "getting the notes."

Homework Policy: Homework is an expectation of the course. The homework problems set by the instructor are to be solved by each group and handed in for grading one day before the class (i.e. till 6pm on the Wednesday before the class). The group members will decide on how to collaborate on solving the problems. Only one homework is needed to be handed in by each group and all the members of the same group will be graded similarly. So, the group members have to be in full coordination. Graded homework will be returned the next day after the lecture. Office hour is set to one day prior to the homework deadline (i.e. 6pm-8pm on Tuesdays) so students can go through any confusion or question about homework with the instructor before this deadline. Each group will solve one problem of their choice in the following class which contributes to the grading of "class participation". It is the responsibility of students to share the solutions of the problems with each other. So, they need to know people in their group and in their class!

Exams: There will be two midterm exams during the semester and one final exam. **Note that all exams will be held online**. Each exam covers the materials discussed during 4 prior lectures.

Midterm Exam I	October 1 (first 4 lectures)
Midterm Exam II	November 5 (second 4 lectures)
Final Exam Period	December 17 (third 4 lectures)

The exams are closed book/notebooks but students are allowed to prepare a double sided A4 page of any material related to class and keep it with themselves during the exam. A picture of this information sheet should be uploaded to Canvas along with the answers to the exam problems.

Makeup Exam Policy: There will normally be **NO MAKE-UP EXAMS** during the semester. In the event that a student has a legitimate reason for missing an exam, the student should contact the Dean of Students office and present written verifiable proof of the reason for missing the exam, e.g., a doctor's note, police report, court notice, etc. clearly stating the date AND time of the mitigating problem. The student must also notify the CES Department Office/Instructor that the exam will be missed so that appropriate steps can be taken to make up the grade.

Cellular Phones: All cellular phones and other electronic devices must be switched off during all class times. Such devices must be stowed in bags during exams or quizzes.

ADDITIONAL RESOURCES

Accommodation of Disabilities: Office of Accessibility Resources and Services (***formerly known as Disability Support Services***) offers long term and temporary accommodations for undergraduate, graduate and visiting students at NJIT.

If you are in need of accommodations due to a disability please contact Chantonette Lyles, Associate Director at the Office of Accessibility Resources and Services at 973-596-5417 or via email at lyles@njit.edu. The office is located in Fenster Hall Room 260. A Letter of Accommodation Eligibility from the Office of Accessibility Resources Services office authorizing your accommodations will be required.

For further information regarding self-identification, the submission of medical documentation and additional support services provided please visit the Accessibility Resources and Services (OARS) website at:

- http://www5.njit.edu/studentsuccess/disability-support-services/

Important Dates See: Fall 2020 Academic Calendar, Registrar
https://www5.njit.edu/registrar/fall-2020-academic-calendar/

Date	Day	Event

September 1	T	First Day of Classes
September 5	S	Saturday Classes Begin
September 7	M	Labor Day
September 8	T	Monday Classes Meet Last Day to Add/Drop a Class Last Day for 100% Refund, Full or Partial Withdrawal
September 9	W	W Grades Posted for Course Withdrawals
September 14	M	Last Day for 90% Refund, Full or Partial Withdrawal No Refund for Partial Withdrawal after this date
September 28	M	Last Day for 50% Refund, Full Withdrawal
October 19	M	Last Day for 25% Refund, Full Withdrawal
November 9	M	Last Day to Withdraw
November 25	W	Friday Classes Meet
November 26	R	Thanksgiving Recess Begins
November 29	Su	Thanksgiving Recess Ends
December 10	R	Last Day of Classes
December 11	F	Reading Day 1
December 14	M	Reading Day 2
December 15	T	Final Exams Begin
December 21	M	Final Exams End
December 23	W	Final Grades Due

Course Outline

Lecture	Date	Topic	Assignment
1	09/03/2020	Introduction to quantum theory	Chapter 1 (4 problems per groups of 4 or 5 students) 1,4,5,6,12,13,16,19,23,24,32,33,34,39,40,42,44,46,48,49
2	09/10/2020	Classical wave equation/Complex numbers	Chapter 2 (2 problems per group) 2,3,4,5,7,11,12,17,18,24,26,28 Mathchapter A (1 problem per group) 1,2,3,4
3	09/17/2020	Schrödinger equation/Probability/Particle in a box	Chapter 3 (2 problems per group) 9,11,12,18,21,22,23,25 Mathchapter B (1 problem per group) problems 1-4

4	09/24/2020	Operators/3D Schrödinger equation/More on probability	Chapter 3 (2 problems per group) 2,3,6,8,29,30,31,35
5	10/01/2020	Midterm exam I (First 4 lectures)	
6	10/08/2020	Postulates of quantum mechanics	Chapter 4 (3 problems per group) 1,3,6,10,16,18,22,26,32,39,43,45
7	10/15/2020	Harmonic oscillator/Vibrational spectroscopy	Chapter 5 (3 problems per group) 2,4,6,13,15,20,22,24,26,29,32,36
8	10/22/2020	Rigid rotator/Spherical coordinate/Rotational spectroscopy	Chapter 6 (4 problems per group) 1,2,5,7,10,12,15,18,20,24,27,30,32,38,39,41 Chaptermath E (1 problem per group) 2,6,9,11
9	10/29/2020	Hydrogen atom	Chapter 7 (3 problems per group) 1,3,5,7,9,12,13,14,18,22,24,27
10	11/05/2020	Midterm exam II (Second 4 lectures)	
11	11/12/2020	Eigenvalue problem: vectors or matrices	Mathchapter C (2 problems per group) 2,4,6,8,10,12,14,16 Mathchapter G (2 problems per group) 2,4,6,8,10,12,14,16
12	11/19/2020	Many-electron atoms	Chapter 9 (3 problems per group). 2,4,7,11,14,18,19,22,24,25,27,28
13	12/03/2020	The chemical bond: one and two-electron molecules	Chapter 10 (2 problems per group) 1,4,8,14,18,26,27,35
14	12/10/2020	Theory of chemical bonding	Chapter 11 (4 problems per group) 5,7,10,11,13,15,16,18,22,24,27,28,35,37,39,41
15	12/17/2020	Final exam (Third 4 lectures)	