Lahore University of Management Sciences

CHEM314: Quantum Chemistry

Fall 2023-24

Instructor	Habib ur Rehman
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Teaching Assistants (TAs)	N/A
TA Office Hours	N/A
Course URL (if any)	LMS

Course Teaching Methodology
• Teaching Methodology: In person. • Lecture Details: Two lectures per week aided by office hours. •

COURSE BASICS				
Credit Hours	3			
Lectures (s)	2	75 min each		
Lab				
Recitation/Lab (per week)				
Tutorial (per week)				

COURSE DISTRIBUTION	
Core	Chemistry Majors
Elective	SSE students at junior/senior level
Open for Student Category	SSE
Closed for Student Category	Non-SSE

COURSE DESCRIPTION
The course starts with discussing some experimental results where classical mechanics failed to provide a satisfactory explanation, which led to a set of new rules and postulates for atomic and sub-atomic level particles in the early twentieth century. It introduces the Schrodinger equation and the necessary mathematics to solve it for a few simple systems. This course then discusses the significance of wavefunctions, operators and eigenvalues, and how a particle's position, momentum and energy are related. SWE will then be solved for harmonic oscillator and the rigid rotator to understand and explain the vibrational and rotational spectra of simple molecules. The exact solution of Schrodinger equation for the hydrogen-like atoms and approximation methods used for the multi-electron atoms are discussed. Periodic properties of elements are discussed in light of the electron-electron repulsion terms, radial distribution functions, the most probable radii shielding and penetration, and the energies of orbitals. This course also discusses the formation of molecular orbitals in molecules from the linear combination of atomic orbitals, to explain bonding theories such as hybridization, MO and Huckel method for conjugated systems.

COURSE PREREQUISITE(S)	
	CHEM101 & Calculus I

COURSE OBJECTIVES

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the students should be able to learn and understand:

- ✓ the failures of classical mechanics in explaining some experimental phenomena and the concept of duality of waves and matter.
- ✓ the properties of operators, wavefunction/eigenfunctions and eigenvalues as applied in quantum mechanics.
- ✓ how to write and solve the Schrodinger equation for simple problems.
- ✓ the properties of wavefunctions and the associated energies for harmonic/anharmonic oscillator and rigid rotator and be able to apply them in understanding the vibrational and rotational spectra of molecules.
- ✓ the quantization of orbital angular momentum and spin angular momentum, and be able to derive the atomic term symbols and relate them with spectroscopic and magnetic properties of atoms/ions.
- ✓ how to relate the probability density, radial distribution functions, most probable radii, nodes, etc with the wavefunctions of various orbitals in hydrogen-like atoms/ions.
- ✓ and appreciate the difficulties in writing the Hamiltonian operators and the Schrodinger equations for multi-electron atoms and the use of approximation methods to solve them.
- ✓ the approaches of a linear combination of atomic orbitals (LCAO) to form molecular orbitals and the formation of hybrid orbitals.
- ✓ the quantum mechanical modeling of □-electrons in conjugated hydrocarbons and aromatic hydrocarbons.

LEARNING OUTCOMES

the students must be able to:

- write and solve the Schrodinger equation for simple systems, and appreciate the ideas of quantization of energy and uncertainty associated with the position of a particle in quantum mechanics.
- relate and apply the vibrational and rotational spectra of molecules with the harmonic/anharmonic oscillator and rigid rotator to get spectroscopic information about the simple molecules.
- estimate the energies and the most probable radii of different orbitals in atoms and use this information to explain the electronic spectra and other periodic properties of elements.
- arrange the σ and π bonding/antibonding molecular orbitals in order of increasing energy in homonuclear diatomic molecules, conjugated hydrocarbons and aromatic compounds, and relate them with their stability and electronic spectra.

GRADING POLICY

Quizzes	25 %	Number of quizzes: 4-6
Assignments	0 %	Number of assignments: 3-6 (these assignments will make 10-20% of quizzes, MT and FE)
Midterm Exam	35 %	
Final Exam	40 %	The instructor has the discretion to change up to 5% of the above grading scheme.

EXAMINATION DETAIL

Midterm Exam	yes
Final Exam	Yes

Harassment Policy

Harassment of any kind is unacceptable, whether it be sexual harassment, online harassment, bullying, coercion, stalking, verbal or physical abuse of any kind. Harassment is a very broad term; it includes both direct and indirect behavior, it may be physical or psychological in nature, it may be perpetrated online or offline, on-campus and off-campus. It may be one offense, or it may comprise of several incidents which together amount to sexual harassment. It may include overt requests for sexual favors but can also constitute verbal or written communication of a loaded nature. Further details of what may constitute harassment may be found in the LUMS Sexual Harassment Policy, which is available as part of the university code of conduct.

LUMS has a Sexual Harassment Policy and a Sexual Harassment Inquiry Committee (SHIC). Any member of the LUMS community can file a formal or informal complaint with the SHIC. If you are unsure about the process of filing a complaint, wish to discuss your options or have any questions, concerns, or complaints, please write to the Office of Accessibility and Inclusion (OAI, oai@lums.edu.pk) and SHIC (shic@lums.edu.pk) —both of them exist to help and support you and they will do their best to assist you in whatever way they can.

To file a complaint, please write to harassment@lums.edu.pk.

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SSE Council of Equity and Belonging
In addition to LUMS resources, SSE's **Council on Belonging and Equity** is committed to devising ways to provide a safe, inclusive and respectful learning environment for students, faculty and staff. To seek counsel related to any issues, please feel free to approach either a member of the council or email at cbe.sse@lums.edu.pk

COURSE OVERVIEW

Week No.	Book	Topic	Book sections	Objectives/ Application
1	Physical Chemistry by McQuarrie	Discovery of electron, Milliken experiment, Rutherford experiment, the demise of classical physics, black body radiation and Planck's quantum hypothesis, photoelectric effect	CH – 1 and lecture notes	Historical background of Quantum mechanics
2	Physical Chemistry by McQuarrie	Bohr model, line spectra of H atom, de Broglie wavelength, wave-particle duality of light and matter, Young's double slit experiment, Heisenberg uncertainty	CH – 1 and lecture notes	wave-particle duality of light and matter
3-4	Physical Chemistry by McQuarrie	The classical wave equation, oscillatory solutions of differential equations, wavefunctions, linear operators, eigenfunctions and eigenvalues, Hamiltonian operator, Schrodinger equations for a free particle, and a particle in 1-D box, quantization of energy states, free-electron model for π-electrons in linear conjugated hydrocarbons	CH – 2 and 3, and lecture notes	Quantum mechanics and quantization of energies.
5-6	Physical Chemistry by McQuarrie	Normalization of wavefunctions, concepts of discrete and continuous probability distributions, probability of finding the particle in a defined interval, uncertainty in momentum and position of a particle in 1-D box and proof of the uncertainty principle, particle in a rectangular well, quantum mechanical tunneling with examples, solution of the Schrodinger equation for a particle in 3-D box, degeneracy of energy states	CH –3, and lecture notes	Applications of Schrodinger equation to some simple systems.
7-8	Physical Chemistry by McQuarrie	Postulates of quantum mechanics, acceptable wavefunctions, representation of classical mechanical variables with quantum mechanical operators, observable quantities and eigenvalues of quantum mechanical operators, time dependent Schrodinger equation, orthogonality of eigenfunctions, operator algebra and commutators. Harmonic oscillator and Hook's law, potential, kinetic and total energies of an harmonic oscillator, harmonic oscillator model for diatomic molecules, harmonic oscillator wavefunctions and Hermite polynomials, anharmonic terms and Morse potential	CH – 4 and 5, and lecture notes	Postulates of quantum mechanics and their applications to harmonic oscillator model for diatomic molecules.
9	Physical Chemistry by McQuarrie	Harmonic oscillator and infrared spectrum, spherical polar coordinates, angular momentum, energy levels of a rigid rotator, rotating diatomic molecules and microwave spectroscopy.	CH – 5, 6, and lecture notes	Harmonic oscillator and rigid rotor
10-11	Physical Chemistry by McQuarrie	Hamiltonian operator for the H atom, Laplacian operator in spherical coordinates, radial and angular equations, spherical harmonics, Legendre polynomials, quantum numbers for the H atom, wavefunctions for various orbitals, probability of finding the electron, radial distribution functions (RDF), calculation of the average and the most probable values of radius in different orbitals, splitting of the energy levels and the Zeeman effect. Schrodinger equation for the He atom, atomic units,	CH – 6, 7 and lecture notes	Solution of Schrodinger equation for H2 and other multi-electron atoms.
12	Physical Chemistry	the variational method with examples, linear combination	CH – 7 and 8, and	Approximation methods,

	by McQuarrie	of trial functions and the secular determinant, perturbation theory, Hartree-Fock equations and the self-consistent field method,	lecture notes	radial distribution functions.
13-14	Physical Chemistry by McQuarrie	spin angular momentum, operators and spin orbitals, Pauli exclusion principle, Russell-Saunders coupling and atomic term symbols, Hund's rules, selection rules and atomic spectra, Born-Oppenheimer approximation, Hamiltonian operator and molecular orbitals of H2+ and H2 molecules, overlap, coulomb and exchange integrals	CH – 8, and lecture notes	Effects of electric and magnetic fields on degeneracy of energy levels
15	Physical Chemistry by McQuarrie	Symmetry labels of molecular orbitals, molecular orbitals of homonuclear diatomic molecules, molecular term symbols, bonding in polyatomic molecules, hybrid orbitals, π-electron approximation for conjugated hydrocarbons and aromatic hydrocarbons, Huckel molecular orbital theory.	CH – 9 and 10	pi-electron approximation for conjugated hydrocarbons and aromatic hydrocarbons

Textbook(s)/Supplementary Readings

Textbook:

1. Physical Chemistry – a molecular approach, D. A. McQuarrie and J. D. Simon, (2008).

Supplementary Readings:

1. Physical Chemistry, Tom Engel , Phil Reid
2. Introduction to Quantum Mechanics, David J. Griffiths
3. Quantum Chemistry and Spectroscopy, Tom Angel
4. Class notes

Examination Detail	
Midterm Exam	- 90 min duration - Mix of Numericals, MCQs, Fill in the Blanks, Short Questions, etc. Closed books, Close notes, only calculators allowed Mobile devices to be switched off during the length of Exam
Final Exam	- 90-120 min duration - Mix of Numericals, MCQs, Fill in the Blanks, Short Questions, etc. Closed books, Close notes, only calculators allowed Mobile devices to be switched off during the length of Exam