Lahore University of Management Sciences

CHEM 511 – Advanced Physical Chemistry

Spring (2023–2024)

Instructor	Falak Sher
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Secretary/TA	N/A
TA Office Hours	N/A
Course URL (if any)	N/A

Course Teaching Methodology (Please mention following details in plain text)

- Teaching Methodology: In-person
- Lecture details: In-person lectures in classroom

Course Basics				
Credit Hours	3			
Lecture(s)	Nbr of Lec(s) Per Week	2	Duration	90 min
Recitation (per week)	Nbr of Rec (s) Per Week	N/A	Duration	N/A
Lab (if any) per week	Nbr of Session(s) Per Week	N/A	Duration	N/A
Tutorial (per week)	Nbr of Tut(s) Per Week	N/A	Duration	N/A

Course Distribution	
Core	MS chemistry students
Elective	SSE Graduate Students
Open for Student Category	
Closed for Student Category	All undergraduate students

COURSE DESCRIPTION

This course covers chemical thermodynamics with focus on the equilibrium properties of macroscopic systems and four fundamental laws of thermodynamics. Calculations involving work, heat, internal energy, heat capacities, enthalpy, entropy, the Gibbs function and chemical potentials are performed. It also covers phase equilibria of single and two component systems, Clausius-Clapeyron equation, ideal/non-ideal solutions, colligative properties.

The second part of the course introduces quantum mechanics and solution of Schrodinger equation for simple systems. It discusses wavefunctions, radial distribution functions, operators and eigenvalues, and how the position, momentum and energy of a particle are related with them in quantum mechanics. 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.

COURSE PREREQUISITE(S)

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No pre-requisite for graduate chemistry students. Undergraduate students are not allowed enroll in this course

COURSE OBJECTIVES

The students should learn

- four thermodynamics laws

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- the equations of states which relate various properties of matter in the gas, liquid and solid phases.
- different forms of energy such as work, heat, internal energy, free energies etc. and their transformation from one form to the other.
- the conditions of spontaneity in physical and chemical processes.
- simple phase diagrams, important relationships describing physical changes from one phase to the other, and characteristics of ideal/non-ideal solutions and effects of temperature, pressure and solute concentrations on their properties.
- the microscopic level understanding of the equilibrium properties of macroscopic systems.
- The failure of classical mechanics in explaining some experimental phenomena and the concept of duality of waves and matter.
- How to write and solve the Schrodinger equation for simple problems.
- 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.
- How to predict periodic properties of elements and describe bonding in simple systems.

Learning Outcomes

The students must be able to

- understand and analyze different forms of energy and their transformations during physical and chemical changes.
- derive correlations using thermodynamic laws and apply them for determining the unknown state functions/properties from the provided information.
- differentiate between spontaneous and no-spontaneous processes from the knowledge of enthalpy and entropy changes at a given temperature.
- apply fundamental principles of thermodynamic and relationships to understand the phase diagrams of simple systems.
- correlate macroscopic equilibrium properties with the microscopic energy levels of molecules in the given system.
- 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.
- 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 □ and □ 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 Breakup and Policy

Assignment(s)/Home Work:	10% (practice questions)
Quiz(s):	20% (7-8 quizzes; mostly announced)
Class Participation:	5%
Attendance:	
Midterm Examination:	25%
Project:	
Final Examination:	40%

Examination Detail

Midterm Exam	Yes/No: Yes Combine Separate: Duration: 90 min Preferred Date:
Final Exam	Yes/No: Yes Combine Separate: Combined Duration: 3 hrs

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COURSE OVERVIEW			
Week/ Lecture/ Module	Topics	Recommended Readings	Objectives/ Application
Week 1	Introduction to thermodynamics, energy, temperature, Boltzmann distribution etc.	Silbey et al and McQuarrie	Energy, temperature and related concepts
Week 2	Work, heat, heat capacities and calculations for different kind of processes	Silbey et al and McQuarrie	Work and heat calculations
Week 3	Internal energy, first law of thermodynamics and related calculations	Silbey et al and McQuarrie	First law of thermodynamics and related problems
Week 4	Enthalpy, constant pressure/volume heat capacity, and temperature and pressure dependence	Silbey et al and McQuarrie	Enthalpy and related calculations
Week 5	Standard enthalpy of reactions and related calculations		Enthalpy of reactions and its temperature dependence
Week 6	Second law of thermodynamics, absolute entropies, third law of thermodynamics	Silbey et al and McQuarrie	Second law of thermodynamics
Week 7	Gibbs free energy and fundamental equations of thermodynamics	Silbey et al and McQuarrie	Fundamental equations of thermodynamics
Week 8	Chemical potential and phase diagrams of single component	Silbey et al and McQuarrie	Phase diagrams
Week 9	Ideal/real solutions, Raoult's law and related calculations	Silbey et al and McQuarrie	Liquid solutions
Week 10	Blackbody radiation, Planck's hypothesis, photoelectric effect, Bohr's atomic model, de Broglie wavelength etc.	Lecture notes	Historical background of quantum mechanics
Week 11-12	Wave function, probability density, Schrodinger equation, particle in 1-D box	Silbey et al and McQuarrie	Introductory quantum mechanics
Week 13	Atomic orbitals, radial distribution functions and orbital energies	Keeler	Orbital energies
Week 14	Periodic table and periodic properties of elements	Keeler	Periodicity

Textbook(s)/Supplementary Readings

Books:

1. Physical Chemistry – a molecular approach, D. A. McQuarrie and J. D. Simon, (2008). & Lecture notes
2. Quantum Chemistry, D. A. McQuarrie (2003)
3. Chemical Structure and Reactivity by J. Keeler and P. Wothers, Oxford Unversity Press
4. Physical Chemistry by R. Silbey, R. Alberty and M. Bawendi ISBN-13: 978-0471215042 (2004).
5. Physical Chemistry, P.W. Atkins

Academic Honesty

The principles of truth and honesty are recognized as fundamental to a community of teachers and students. This means that all academic work will be done by the student to whom it is assigned without unauthorized aid of any kind. Plagiarism, cheating and other forms of academic dishonesty are prohibited. Any instances of academic dishonesty in this course (intentional or unintentional) will be dealt with swiftly and severely. Potential penalties include receiving a failing grade on the assignment in question or in the course overall. For further information, students should make themselves familiar with the relevant section of the LUMS student handbook.

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Harassment Policy
There is absolutely zero tolerance for any behaviour that is intended, or has the expected result of making anyone uncomfortable and negatively impacts the class environment, or any individual's ability to work to the best of his/her potential. In case a differently-abled student requires accommodations for fully participating in the course, students are advised to contact the instructor so that they can be facilitated accordingly. If you think that you may be a victim of harassment, or if you have observed any harassment occurring in the purview of this class, please reach out and speak to the instructor. If you are a victim, it is strongly encouraged to reach out to the Office of Accessibility and Inclusion at *oai@lums.edu.pk* or the sexual harassment inquiry committee at *harassment@lums.edu.pk* for any queries, clarifications, or advice. You may choose to file an informal or a formal complaint to put an end to offending behaviour. You can find more details regarding the LUMS sexual harassment policy at: *https://mgshss.lums.edu.pk/lums-harassment-policy*. To file a complaint, please write to *harassment@lums.edu.pk*. 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 issue, please feel free to approach either a member of the council or email at *cbe.sse@lums.edu.pk*.