Lahore University of Management Sciences

CHEM 313: Special Topics in Physical Chemistry

Spring 2024

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TA Office Hours	N/A
Course URL (if any)	LMS

Course Teaching Methodology
• Teaching Methodology: In-person • Lecture details: Mostly on board with some lectures on PowerPoint slides

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 – consent required from the instructor
Open for Student Category	
Closed for Student Category	

COURSE DESCRIPTION
This course will expose students to core concepts in physical chemistry building on the fundamentals covered in earlier courses and extending these concepts to the areas of chemical kinetics and statistical thermodynamics.

COURSE PREREQUISITE(S)	
	None

COURSE OBJECTIVES
Objective of this course are to: • Broaden and deepen the overall knowledge of physical chemistry • Specifically increase the understanding of the basic concepts in chemical kinetics and statistical thermodynamics • Increase the capability to successfully apply the acquired knowledge to solve chemical problems • Enhance the analytical skills in problem solving capabilities

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LEARNING OUTCOMES
On the completion of this course students should be able to: • Clearly understand the fundamental principles of statistical mechanics and thermodynamics • Derive thermodynamic properties using partition functions • Distinguish between zero-, first-, and second-order reactions

GRADING POLICY		
Quizzes	20 %	Number of quizzes: 7 – 8
Mid-Term Exam	30 %	
In-class presentations	10 %	
Final Exam	40 %	

EXAMINATION DETAIL	
Midterm Exam	Yes (75 min in class)
Final Exam	Yes (180 min)

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 behaviour, 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 favours 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.

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	Topics	Recommended Readings	Objectives/ Application
	Chemical Kinetics		
1-2	Kinetic theory of gases, pressure of an ideal gas, rms speed, Maxwell-Boltzmann distribution of molecular velocities, molecular collisions	**[SR]** and Lecture notes	Maxwell-Boltzmann speed distribution, mean free path and collision frequency
3	Rate laws for different reaction orders, determining rate laws experimentally	**[SR]** and Lecture notes	Kinetic studies from experimental data
4-6	Effect of temperature on reaction rates, Arrhenius equation, collision theory, reaction mechanisms, steady-state approximation, catalytic reactions, Isotope effect	**[SR]** and Lecture notes	Understanding reaction mechanisms and rate limiting steps
7	Introduction to surface chemistry and reactions on surfaces	Lecture notes	Understanding the role of surfaces in catalytic reactions
	Statistical Thermodynamics		
8	Introduction to probability and statistics, Overview of Series, approximations, multivariate calculus and distribution functions	**[KD]** and lecture notes	To learn basic mathematical tools for development of statistical thermodynamics

9	Extremum principles and Boltzmann entropy, microscopic view of entropy	**[KD]** and lecture notes	To learn how systems tend towards states with minimal energies or maximal multiplicities in context of first and second law of thermodynamics
10-11	The Boltzmann distribution law, partition functions, prediction of thermodynamic properties from partition functions,	**[KD]** and lecture notes	To learn about partition function and computation of thermodynamics and averaged physical properties
12-13	Statistical mechanics of simple gases and solids, other applications.	**[KD]** and lecture notes	Use of quantum level energy levels to predict the thermodynamics properties of gases and simple solids (particle-in-a-box model, harmonic oscillator model, rigid-rotor model, Einstein model)
14	Specific heat capacity: Einstein crystal and Debye crystal	**[KD]** and lecture notes	Use of the non-interacting quantum harmonic oscillator model and the phonon model to estimate the specific heat capacity of solids

Textbook(s)/Supplementary Readings

[SR] Silbey, R., R. Alberty, and M. Bawendi. *Physical Chemistry*. 4th ed. New York, NY: John Wiley & Sons, 2004. ISBN: 9780471215042. Part 3 (Kinetics).
[PH] Houston, P. *Chemical Kinetics and Reaction Dynamics*. New York, NY: McGraw-Hill, 2001. ISBN: 9780072435375.
[DM] Donald A. McQuarrie and John D. Simon. *Physical Chemistry: A Molecular Approach*. Chapters 25, 26, 27.
[AP] Atkins, P., and J. de Paula. *Physical Chemistry*. 7th ed. New York, NY: W.H. Freeman and Company, 2001. ISBN: 9780716735397.
[KD] Ken A. Dill and Sarina Bromberg. *Molecular Driving Forces: Statistical Thermodynamics in Biology, Chemistry, Physics and Nanoscience*. 2nd ed. London and New York: Taylor & Francis Group, 2010. ISBN: 9780815344308.
[DS] An Introduction to Thermal Physics, Daniel V. Schroeder.