Physical Chemistry I Chemistry 3750 Fall 2020

General Information

Time: MWF 8:15-9:10 a.m.

Zoom Meeting ID: 932 4304 8857 Passcode: PChem3750

Course Summary

An introduction to physical chemistry, concentrating on quantum mechanics, group theory and spectroscopy.

D2L Site

A Desire2Learn (D2L) site (http://elearn.etsu.edu) for this course is available. All assignments, handouts, etc. will be posted to the site.

Contact Information

Instructor: Dr. Scott Kirkby Phone: 423-439-8638 Office Hours: By appointment (virtual) Office: 464 D. M. Brown Hall Email: kirkby@etsu.edu

Individual assistance may also be obtained by emailing questions to the instructor.

Text

McQuarrie, D. A. and Simon, J. D. Physical Chemistry, A Molecular Approach, University Science Books, Sausalito, California 1997. A solution manual for the text is also available: Cox, H. Problems and Solutions to Accompany McQuarrie and Simon Physical Chemistry, A Molecular Approach; University Science Books, Sausalito, California 1997.



Grading

Assignment	Percent of Final Grade
Problem Sets, Quizzes & Assignments	25%
Take-Home Midterm Tests (10% each)	
Week of 1 October	
Week of 1 November	20%
22 November	
3MT Style Zoom Presentation	
10% peer evaluation	20%
10% instructor evaluation	
Final Exam (Take-Home)	
Wed. 9 Dec.	40%
Total	100%

The midterm tests will not be explicitly cumulative, but material from previous tests may be required to complete the current work. There will be no make-up tests except for extenuating circumstances. Written documentation (*e.g.* a doctor's note) must be provided. If you must miss an exam, arrangements should be made with the lecturer before the exam. The remaining midterm and the final exam will still compose 60% of your grade. The final exam will be comprehensive.

Academic Integrity

This course will comply with the Department of Chemistry's Academic Integrity Policy (available in the course's content section on D2L). Any violation of the policy is unacceptable and will not be tolerated. At the minimum, a grade of zero for the assignment will be given.

3MT Style Zoom Presentation

Working individually, students will prepare a one slide, three (3) minute Zoom presentation in the style of a 3MT virtual presentation (https://threeminutethesis.uq.edu.au/) on any topic in quantum mechanics or spectroscopy. An important difference is that these will be live, on Zoom, rather than recorded. As intermediate steps in the preparation of the presentation, an abstract of the topic must be submitted by 16 October, a draft of the slide must be submitted by 6 November, and the final version of the slide by 30 November. The presentations will take place during the final two lectures in December. Grading of the presentations will be by the other students and the instructor.

Conversion to Letter Grades

Grade	Percent	Grade	Percent
А	$\geq 90.00\%$	С	63.00 - 66.99%
A-	85.00-89.99%	C-	60.00 - 62.99%
B+	80.00 - 84.99%	D+	55.00 - 59.99%
В	75.00 - 79.99%	D	50.00 - 54.99%
B-	70.00 - 74.99%	F	<50.00%
C+	67.00 - 69.99%		

This course is an introduction to physical chemistry. The material is often very abstract and highly mathematical. It cannot be learned the night before a test. It can only be mastered by working problems. Please make every attempt to keep up and do not hesitate to ask questions both in and out of class.

Practice Test Problems: A set of practice test problem has been posted to the D2L site. The solutions, with annotations explaining the awarding of points, have been posted as well.

Lecture Titles

- 1. The Denouement of 19th Century Classical Mechanics
- 2. Planck's Quantum Hypothesis and the Hydrogen Atom Spectrum
- 3. de Broglie's Postulate and the Heisenberg Uncertainty Principle
- 4. The Classical Wave Equation: Model for a One Dimensional Vibrating String
- 5. The Schrödinger Equation
- 6. Particle in a Box: A Mathematical Model for One Particle Problems
- 7. Electrons in a Box: A Model for Conjugated Polyenes
- 8. Postulates and Principles of quantum Mechanics
- 9. The Time-Dependent Schrödinger Equation
- 10. Putting it All Together: Selected Particle in a Box Problems
- 11. The Classical Harmonic Oscillator
- 12. The Quantum Mechanical Oscillator
- 13. Harmonic Oscillator Wave Functions Hermite Polynomials
- 14. The Rigid Rotator
- 15. The Schrödinger Equation for the Hydrogen Atom
- 16. Wave Functions for the Rigid Rotator
- 17. Hydrogen Atomic Orbitals
- 18. The Variational Method
- 19. Perturbation Theory
- 20. Selected Problems From Our Model Systems
- 21. An Approximate Solution for the Helium Atom
- 22. Multielectron Atoms and the Hatree-Fock Method
- 23. Electron Spin
- 24. Atomic Spectra, Term Symbols and Hund's Rules
- 25. The Born-Oppenheimer Approximation and the Chemical Bond
- 26. Bonding is a Quantum Mechanical Phenomenon

- 27. Molecular Orbital Theory
- 28. Molecular Term Symbols
- 29. Bonding in Polyatomic Molecules
- 30. Why is Water Bent? Delocalized Bonding
- 31. Selected Problems: Multielectron Systems
- 32. Group Theory The Exploitation of Symmetry
- 33. Molecular Spectroscopy

Note: You will also be responsible for all of the mathematics covered in Math Chapters A-F.

Course Notes

Course notes and lecture slides will be available for download from the course D2L site. These are not meant to be a complete set, merely an additional aid to the student. No assurances are given for their correctness. The textbook should be assumed to be correct in all conflicts between it and these materials.

Suggested Problems

Chapter 1: 1, 3, 8, 12, 15, 17, 22, 23, 26, 37, 38, 42 Chapter 2: 1, 3, 5, 6, 7, 9, 10, 13, 16, 18, 20, 21 Chapter 3: 1, 2, 3, 7, 10, 11, 17, 22, 27, 28, 29, 34 Chapter 4: 1, 3, 4, 5, 8, 10, 11, 16, 19, 33, 35, 38 Chapter 5: 4, 5, 7, 13, 14, 18, 19, 21, 25, 37, 45, 47 Chapter 6: 1, 4, 10, 17, 18, 20, 22, 24, 26, 34, 46, 47 Chapter 7: 2, 3, 7, 8, 11, 15, 18, 20, 21, 24, 28, 29 Chapter 8: 1, 3, 5, 10, 19, 22, 26, 28, 30, 31, 39, 47 Chapter 9: 1, 2, 8, 9, 12, 13, 14, 19, 25, 26, 32, 40 Chapter 10: 1, 2, 5, 7, 8, 10, 19, 21, 31, 32, 37, 47 Chapter 12: 1, 2, 3, 4, 9, 11, 14, 18, 24, 27, 31, 36 Chapter 13: 1, 2, 3, 7, 11, 12, 14, 16, 20, 27, 38, 49

Note: Students are encouraged to attempt as many problems as required to become proficient with the course material in addition to those listed above. Questions at the end of each chapter in the text are numbered in the format: chapter number - question number, the question number above corresponds to the number in the given chapter.

Sample Midterms and Final

Three sample midterm tests and a final exam have been posted to the D2L site.

Lab Safety Training

If you are enrolled in laboratory courses (*e.g.* CHEM 3611) you are required to complete the mandatory safety training module. Please contact your lab instructor for details.

Disability Services

It is the policy of ETSU to accommodate students with disabilities, pursuant to federal law, state law and the University's commitment to equal educational access. Any student with a disability who needs accommodations, for example arrangement for examinations or seating placement, should inform the instructor at the beginning of the course. Faculty accommodation forms are provided to students through Disability Services located on the upper level of the D.P. Culp Center (Suite 390), telephone 439-8346.

Mental Health

Students often have questions about mental health resources, whether for themselves or a friend or family member. There are many resources available on the ETSU Campus, including: ETSU Counseling Center (423) 439-4841; ETSU Behavioral Health & Wellness Clinic (423) 439-7777; ETSU Community Counseling Clinic: (423) 439-4187.

- If you or a friend are in immediate crisis, call 911.
- Available 24 hours per day is the National Suicide Prevention Lifeline: 1-800-273-TALK (8255).