

# Physical Chemistry I

## Chemistry 3750

### Fall 2018

#### General Information

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

Place: 265 D. M. Brown Hall

#### 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: Monday, 10:00 a.m. - 12:00 noon

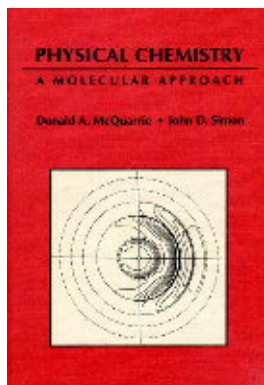
Office: 464 D. M. Brown Hall

Email: [kirkby@etsu.edu](mailto:kirkby@etsu.edu)

Individual assistance may also be obtained by appointment or 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   | 10%                    |
| Best Two of Three Midterm Tests<br>17.5% each (1 hour, in class)<br>28 September<br>26 October<br>30 November | 35%                    |
| Poster Presentation<br>10% peer evaluation<br>5% instructor evaluation  | 15%                    |
| Final Exam (2 hours)<br>Wed. 13 Dec.,<br>3:50 - 5:50 p.m.   | 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. An early ride home, being late for class, *etc.* are not such circumstances. If you must miss an exam, arrangements should be made with the lecturer before the exam. If you miss more than one midterm, the remaining midterm and the final exam will still compose 65% of your grade.

**Calculators:** Non programmable scientific calculators are permitted for use on the midterm tests and the final exam. Programmable calculators may not be used. Calculators that are part of a communications device, including IR transmitting calculators, are not permitted.

**Cell Phones, *etc.*:** Cell phones, pagers, IR transmitting calculators or any other communications devices are not permitted during tests or the final exam. Use of any communications device during a test or final will result in a grade of zero for the assignment. For the purposes of this course, possession in a functional state will be considered usage.

## 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.

## Poster Presentation

Working in pairs, students will prepare a poster, in the style of a scientific poster, on any topic in physical chemistry. These posters will be presented at the end of term. As intermediate steps in the preparation of the poster, an abstract of the topic must be submitted by 17 October, and a "story board" or equivalent outline must be submitted by 9 November. Grading of the posters will be by the other students and the instructor.

## Conversion to Letter Grades

| Grade | Percent        | Grade | Percent        |
|-------|----------------|-------|----------------|
| A     | $\geq 90.00\%$ | C     | 63.00 - 66.99% |
| A-    | 85.00-89.99%   | C-    | 60.00 - 62.99% |
| B+    | 80.00 - 84.99% | D+    | 55.00 - 59.99% |
| B     | 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 Hartree-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 will be available for download from the course D2L site. These notes 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 notes.

## 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 online safety training module. This is available on D2L at the ADMN-0005-573 - Chemistry Safety Quiz site. You must complete and pass the on-line quiz once

a year before being allowed in lab. If you do not complete the safety training prior by 4:30 p.m. on Friday 31, August 2018, you will not be allowed to remain in these classes.

## **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 third floor of Nell Dossett Hall, 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).