

# Quantum Chemistry

## Chemistry 5743

### Fall 2011

#### General Information

Time: MW 7:00-8:20 p.m.

Place: 476 D. M. Brown Hall

#### Course Summary

An introduction to quantum mechanics with emphasis on the concepts and mathematical methods closely related to chemistry. Prerequisites: One year of physical chemistry requiring calculus.

#### 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: 423-439-5823

Office Hours: Mon., 9:30-11:30 a.m.

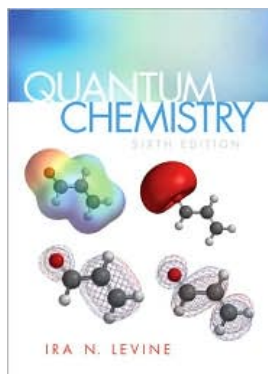
Office: 464 D. M. Brown Hall

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

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

#### Text

Levine, I. N. Quantum Chemistry 6th Ed., Pearson Prentice Hall, Upper Saddle River NJ, 2009.



## Grading

Assignment	Percent of Final Grade
Problem Sets & Assignments	20%
Best Two of Three Midterm Tests 15% each (1 hour, in class) 26 September 26 October 28 November	30%
Poster Presentation 5% peer evaluation 10% instructor evaluation	15%
Final Exam (2 hours) Mon. 12 Dec., 8:10 - 10:10 p.m.	35%
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.

## Presentation

Each student will prepare a short (approximately 20 minutes) presentation, in the style of a scientific talk, on any topic in quantum mechanics. These will be presented at the end of term. As intermediate steps in the preparation of the talk, an abstract of the topic must be submitted by 12 October, and a "story board" or equivalent outline must be submitted by 14 November. Grading of the talks will be by the other students and the instructor. Participation in peer grading is mandatory. Failure to participate will result in the loss of the peer grade.

## Conversion to Letter Grades

Grade	Percent	Grade	Percent
A	$\geq 90.00\%$	B-	70.00 - 74.99%
A-	85.00-89.99%	C+	65.00 - 69.99%
B+	80.00 - 84.99%	C	60.00 - 64.99%
B	75.00 - 79.99%	F	$<60.00\%$

## Lecture Topics

1. Introduction
2. The Schrödinger Equation
3. Particle in a Box
4. Operators
5. The Harmonic Oscillator
6. Angular Momentum
7. The Hydrogen Atom
8. Theorems of Quantum Mechanics
9. The Variation Method
10. Perturbation Theory
11. Additional topics as time permits

**Note:** You will also be responsible for all of the mathematics covered.

## Suggested Problems

Students are encouraged to attempt as many problems as required to become proficient with the course material.

## Sample Midterms and Final

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

## 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).