CHM 4412 – Physical Chemistry – Quantum Chemistry and Spectroscopy

Instructor: Gail E. Fanucci
Phone : 352-392-2345
E-mail: fanucci@chem.ufl.edu
Class Times: T,R 2+3 (8:30-10:25)
Office Hours: Monday, 7th period
Thursday, 4th period
Location: CLB 311F/313 (check my office, 311F first. We will use 313 if large numbers of people show up for help.

Text: Physical Chemistry, 9th Ed Atkins.
(you can use other texts for reading materials; however homework problems will be assigned from book. I will try to post scanned copies on Sakai, but it is in your interest to get a copy or share with a classmate or use the library reserved copy).

Purpose: The purpose of this course is to achieve knowledge of the microscopic physical chemistry of molecules sufficient to enable one to continue studies in quantum mechanics, atomic and molecular structure, symmetry, and spectroscopy.

Homework: Homework sets will be assigned and graded. Homework will not be weekly, but one homework set per exam material will be given and graded.
Quizzes: There will also be 3 on-line quizzes that will be meant to aid your study for exams. You will have an infinite number of times to attempt the quiz.
Due Dates for Homework, Quiz Dates and Exam Dates will be posted on Sakai.

Points Earnable:

4 progress exams	200 pts each	800 pts
4 homework	50 pts each	200 pts
3 quizzes	50 pts each	150 pts
In class participation	50 pts	50 pts

Total: 1200 pts

Grading Scale: The following grading scale is tentative, and could be adjusted to be less stringent. The scale will not be more difficult.

Points	Percentages	Grade
1116-1200	93% ≥	A
1068-1115	89% - 92.5%	A-
1020-1114	85% - 88.5%	B+
960-1019	80% - 84.5%	B
900-959	75% - 79.5%	B-
840-899	70% - 74.5%	C+
780-839	65% - 69.5%	C
720-779	60% - 64.5%	C-
660-719	55% - 59.5%	D+
600-659	50% - 54.5%	D
559-0	> 50%	E

1. Exam Policies: Four exams will be given. These will be during class times and will not be cumulative. There is no final exam. Exams will be roughly 2 hours. NO GRAPHING CALCULATORS will be allowed. You will need a calculator for taking the exam. No sharing of calculators will be allowed. No cell phones will be allowed while taking an exam. You will be given the relevant equations and constants, units and integrals if necessary. Making up a missed exam is a serious and exceptionally burdensome problem. Consequently, a make up exam will be granted solely at the discretion of the instructor. This will require that you have a legitimate excuse and that you have brought this to the attention of the instructor before missing an exam (and hopefully not the day before!). Legitimate excuses include sickness and deaths of close family members, travel to national conferences (proof of travel required) etc. Please discuss the excuse with me before assuming a make up will be granted. A student contending that an exam has been misgraded or misscored must report this to the instructor or TA responsible for grading within one week of receiving the original grade or score. Failure to follow this procedure results in no reconsideration of the contended grade or score. For all questions on grading or scoring please consult with the TA or instructor in person. For on-line quizzes emailed questions on grading or absences will not be answered.

2. On-line quizzes: There will be three on-line quizzes on Sakai. The on-line quizzes will be available for a certain amount of time and can be repeated indefinitely. The quizzes are intended to be a study guide to help prepare you for studying for the exam.

3. Homework: There will be assigned problems to be turned in for grade. You must show your original work and all of the work for full credit. At times, problems may be assigned where the answer is given in the back of the book. You must show your work for full credit. Again, the point of the homework is to help guide you to prepare for the material you will be tested on. At times the homework may be more extensive than the problems that appear on exams. Exams are only 2 hours long; they cannot test you on every homework problem that you have done.

4. Prerequisites: Technically CHM4411 and MAC 2313. I do not believe 4411 is a prerequisite and if you have not taken CHM4411 you should be at no disadvantage. However, physical chemistry is a subject that makes extensive usage of mathematics; in particular differentiation, integration, basic differential equations and some matrix algebra. You should make some effort to freshen up your mathematics background for this course. Throughout the semester important mathematical concepts will be reviewed or introduced. Obviously if you have taken an "advanced" math class such as Differential Equations or Matrix Algebra; many of these topics will seem basic. However, without a formal course in these areas, the mathematics may become challenging. You should feel welcome to ask questions during office hours of the TA and me for help with mathematics concepts.

5. Study Habits: This course requires an average of 6-8 hours/week of work outside the class. Regular lecture attendance is essential. Although the course follows the book, I use other text books for alternative explanation and examples to complement the material found in the Atkins text book (Engle, McQuarrie, Levine). The notes are intended to help you better understand the material when you read the Atkins text book and work on homework problems. It is expected that you read the material before hand. Although some class notes and handouts will be made available on line; this material is best learned through explanations, working problems and asking questions when you do not understand. This material is often considered one of the more difficult courses you will take and it requires you to stay on top. Although there is no formal cumulative exam, the concepts learned in Chapters 7 and 8 are essential to those in 9 and 10!

6. Students with disabilities: Students requiring special accommodations should register with the Dean of Student Offices and present documentation from that office to the instructor

7. Counseling Services: The University of Florida provides counseling services for students, staff, and faculty. See http://www.counsel.ufl.edu/ or call (352)-392-1575 during regular service hours (8am-5pm). For other hours or weekends call the Alachua County Crisis Center (264-6789). Students may also call the clinician on-call at Student Mental Health for phone callback and consultation at (352)-392-1171.

8. Cell phones: Please put all cell phones or pagers on "silent mode" and in your backpacks or purse during all class periods. No texting, internet searching, tweeting or face book activities during lecture.

9. Honor Code: This class will operate under the policies of the student honor code which can be found at http://www.registrar.ufl.edu/catalog/policies/students.html The students, instructor and TAs are honor bound to comply with the Honors Pledge: We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity.

Obviously study groups to work on homework and quizzes are encouraged. This does not mean it is acceptable to copy the work of your classmates. If you have questions, please ask.

Cheating on an exam will result in a grade of zero for that case. If any homework assignment is suspect, a grade of zero will also be given for that assignment.

Topic Outline and Tentative Schedule:

Exam 1 Topics:

Quantum Theory: Introduction and principles
- -The origins of Quantum Mechanics
- -The dynamics of microscopic systems
- -The Quantum Mechanical principles

Quantum Theory: Techniques and applications
- -Translational Motion
- -Vibrational Motion
- -Rotational Motion

Exam 2 Topics:

Atomic Structure and spectra
- -The structure and spectra of Hydrogenic atoms
- -The structures of many-electron atoms
- -The spectra of complex atoms

Molecular Structure
- -The Born-Oppenhiemer approximation
- -Valance-bond theory
- -Molecular Orbital (MO) Theory
- -Molecular orbitals for polyatomic systems

Exam 3 Topics:

Molecular Symmetry
- -Symmetry elements
- -Applications to MO theory and spectroscopy

Molecular Spectroscopy 1: Rotational and vibrational spectra
- -Pure rotational spectra
- -The vibrations of diatomic molecules
- -The vibrations of polyatomic molecules

Molecular Spectroscopy 2: Electronic transitions
- -The characteristics of electronic transitions
- -The fates of electronically excited states

Molecular Spectroscopy 3: Magnetic Resonance
- -The effect of magnetic fields on electrons and nuclei
- -Electron Paramagnetic Resonance (EPR) Spectroscopy

Exam 4 topics:

Molecular Spectroscopy 3: Magnetic Resonance (continued)
- -Nuclear Magnetic Resonance (NMR) spectroscopy
- -Pulse techniques in NMR

Statistical Thermodynamics 1: The concepts
- -The distribution of molecular states
- -The internal energy and the entropy
- -The canonical partition function

Statistical Thermodynamics 2: Applications
- -Fundamental relation using statistical thermodynamics