

## CHM4412 QUANTUM CHEMISTRY & SPECTROSCOPY

THE CLASS COVERS MATERIAL TO LEARN ABOUT FUNDAMENTAL PHYSICAL PROPERTIES WHICH ARE THE BASE FOR UNDERSTANDING CHEMICAL AND PHYSICAL BEHAVIOR OF MATTER AS WELL AS FUNDAMENTAL CONCEPTS OF SPECTROSCOPY.

### Instructor:

Professor Valeria Kleiman. 311B CLB (Chemistry Laboratory Building), e-mail: [kleiman@chem.ufl.edu](mailto:kleiman@chem.ufl.edu), phone: 392-4656

Teaching Assistant: Hugo Marroux [hmarroux@gmail.com](mailto:hmarroux@gmail.com)

To contact regarding private information (grades, etc) use the SAKAI e-mail option

### Class Schedule:

Spring Semester 2012: August 22<sup>st</sup> - December 14<sup>th</sup>.

T, R Period 2-3 (8:30 - 10:25 am) @ Leigh 207

### Office Hours:

Prof Kleiman: T (1:00-2:00pm) , F )10:30-11:30 pm) in CLB 313. At any other time, send e-mail for an appointment.

Hugo Marroux: M: 6:00-7:00 pm, W: 9:00-10:00 am F: 1:30-2:30 pm CLB 311 At any other time, send e-mail for an appointment.

### Prerequisites:

This class makes extensive use of mathematics (integration, differentiation, matrix algebra, graphing) If you are not up to speed in your math skills, you should work on that in the first week of the semester. Be sure you feel comfortable with these concepts so you can concentrate on the physical chemistry (see HW 0). You can ask question to the TA or the instructor at any point thorough the semester. **MAC 2313 is a prerequisite**, CHM4411 is not.

### Textbook:

The material we cover is available on any Quantum Chemistry textbook for undergraduate level students. I used to assign a particular book, but some students would like it while others would hate it. Below is a list of possible books. In addition, I will provide extensive notes through the SAKAI site. You can use the notes to see the topics we cover and go to ANY of the listed books for more "in-depth" reading. From time to time I will provide some additional reading too.

List of possible books (in random order):

**Principles of Physical Chemistry** by Lionel Raff (very detailed)

**Quanta, Matter and Change** by P. Atkins, J de Paula and R. Friedman (not as detailed, but good conceptually)

**Quantum Chemistry and Spectroscopy** (2nd Ed) by T. Engel (used it in the past, some liked it, some hated it)

**Physical Chemistry** (9th Ed.) by P. Atkins (used it in the past, some liked it, some hated it)

### Attendance:

Attendance to lectures and office hours is expected. In many instances (and as time allows), the 2-period class will combine a traditional lecture with discussion of problems. Reading the material BEFORE lecture time is paramount to keep up with the fast pace of the course. In addition to the 4 hrs class a week, 10-12hrs /week of reading,

homework and general study are required (this is according to previous students who took the course).

## Course Web Site:

We have a course workspace in SAKAI (<http://lss.at.ufl.edu/>). The site will have copies of the syllabus, homework assignments, quizzes, and exams. It will also serve as a communication tool between the instructor and you. If you are register for the course, you are automatically registered in Sakai.

## Homework:

Homework due date is posted on the class calendar. Late homework (if it is turned in on the same day, but after deadline) will have a **20% deduction on the grade**. The day after, the solutions will be posted, and no more homework will be accepted for grading. Each homework problem has to show the **full derivation**, using SI units. **No points will be given for a final result without justification.**

## Exams and quizzes:

There will be 3 progress exams. Conflicts with these exams dates (travel to conferences, visiting graduate schools) must be resolved with the instructor no later than 5 days prior to the exam date. Emergency situations (sickness, death in the family, etc) have to be communicated to the instructor within 48 hrs of the exam and will be considered at the discretion of the instructor.

There will be no make-up exams.

Quizzes are meant to help you study. Throughout the semester, there will be quizzes administered through SAKAI.

## Course Grading:

The grade will be determined by homework (25%), Quizzes (15%), Exams (50%), and in-class participation (10%).

If after the last progress test your grade is above 80% you'll be given the opportunity to skip the final exam (details to be explained in class). If you take the final, the grade will be included in the Exams portion with a 30% weight.

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

## Honor Code:

The student honor code 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.*

## Students with disabilities:

Students requiring special accommodations need to register at the Dean of Student Offices and bring the documentation to the instructor.

Counseling services are available at <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.

## Class schedule:

This is a **tentative** schedule for the course. If changes are made, they will be announced via Sakai

Dates	Topic	Reading/HW
Aug 23-28	Introduction to Quantum Theory	HW 0 due Aug 31

		Reading 2.1, 2.2 Watch 2.11
Aug 30-Sept 4	Postulates, Free particle, 1D box	Read 2.3 3.1
Sept 6-11	Real World Applications, Operators Theory	Read 3.2 3.3
Sept 13 -18	Operators, Harmonic Oscillator	
Sept 20-25	Angular Momentum	
Sept 27	H Atom	
<b>Monday, October 1st EXAM 1 includes up to Angular Momentum</b>		
Oct 2	H Atom	
Oct 4	Spin	
Oct 9-11	Many e-atoms	
Oct 16-18	Molecules (Diatomics)	
Oct 23	Molecular Symmetry	
<b>Wednesday Oct 24 (or Monday Oct 29) EXAM 2 includes up to Diatomic molecules</b>		
Oct 25	Molecular Symmetry	
Nov 1-6	Polyatomic Molecules	
Nov 8-13	Diatomic Spectra	
Nov 15-20	Electronic Spectra	
Nov 27-29	Magnetic Resonance Spectra EPR	
Dec 4	Applications	
<b>Wednesday Dec 5th EXAM 3 includes up to Applications</b>		
<b>Comprehensive Final Date to be discussed</b>		