

## CHM 4412: QUANTUM MECHANICS AND 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: Lauren McCarthy and Alejandra Hermosilla-Palacios

### Class Schedule:

Fall Semester 2014: August 24 – December 9. T, R Period 2-3 (8:30 am– 10:25 pm) @ Weil XXX

No class on Nov 11, Nov 26

### Office Hours:

There is an opportunity to attend office hours every day of the week. If by luck you cannot attend ANY of the available times let me know the first week of class.

Prof Kleiman: Tuesdays 11:00 am -12:00 pm) CLB 311B At any other time, send e-mail for an appointment.

I have an open door policy, so stop by my office and see if I'm available.

T.A. (it might be changed after the 1<sup>st</sup> week of classes): M 5 period, W 8-period R 10- period and F 9- period

### Prerequisites:

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

**MAC 2313 is an important prerequisite**, CHM4411 is NOT a prerequisite.

### Textbook:

The material we cover is available on any Quantum Chemistry textbook for undergraduate level students. I will provide extensive notes through the class web 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 (follow this link for [student feedback on the books](#) ):

**Physical Chemistry, a Molecular Approach** by D. McQuarrie (Students with a good math background will truly enjoy this book. Very complete)

**Physical Chemistry** by P. Atkins (some students like it, others do not)

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

**Quantum Chemistry and Spectroscopy** by T. Engel (some students like 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, ~8/week of reading, homework and general study are required.

## Course Site:

We have a course workspace (<http://lss.at.ufl.edu> ([Links to an external site.](#))). it contains ALL the information about the course, including 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, although you are still responsible to finish it to be ready for the exams. Each homework problem has to show the **full derivation**, using SI units. **No points will be given for a final result without justification.**

## Graphing Software:

This class requires a considerable amount of graphing. This must be done professionally and formatted for presentation in an ACS journal. You can use Matlab (free in UF comp. labs and as an [App \(Links to an external site.\)](#)), Origin, Igor, GRACE (free), gnuplot (free), or any other software of your choice. You will need time to learn to use it, so plan ahead. You must be able to have full control of axis, symbols, lines, and colors, be able to do linear fitting, learn to plot multiple dataset on the same graph, multiple graphs printed in a single page, etc.

## Quizzes:

Throughout the semester, there will be quizzes administered through the class website. Quizzes are meant to help you study. They are announced during class and are added to the calendar.

## Exams:

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.

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

## Course Grading:

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

There is NO FINAL in this class. **If after the last progress test your grade is in peril, you'll be given the opportunity to take a comprehensive exam.**

*Cheating on an exam will result in a grade of zero. Although homeworks are expected to be worked "in group", the submitted homework solution must be **your individual** work. 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.

## Tentative Schedule of Lectures (as of august 24th)

| Dates                                          | Topic                                                             |
|------------------------------------------------|-------------------------------------------------------------------|
| Aug 25 -27                                     | <a href="#">Introduction to Quantum Theory/ Scientific Method</a> |
| Sept 1-3                                       | <a href="#">Postulates, Free particle, 1D box</a>                 |
| Sept 8- 10                                     | <a href="#">Applications Of particle in a box, Operators</a>      |
| Sept 15-17                                     | <a href="#">Harmonic Oscillator</a>                               |
| Sept 22-24                                     | <a href="#">Angular Momentum</a>                                  |
| Sept 29                                        | <a href="#">Angular Momentum</a>                                  |
| Oct 1-6                                        | <a href="#">H atom</a>                                            |
| <b>October 6th TENTATIVE: (evening) EXAM 1</b> |                                                                   |

|                                                                                               |                                                   |
|-----------------------------------------------------------------------------------------------|---------------------------------------------------|
| (includes up to Angular Momentum)                                                             |                                                   |
| Oct 8                                                                                         | <a href="#">Spin</a>                              |
| Oct 13-15                                                                                     | <a href="#">Atoms with many e-</a>                |
| Oct 20-22                                                                                     | <a href="#">Diatomic molecules</a>                |
| Oct 27-29                                                                                     | <a href="#">Molecular Symmetry</a>                |
| <p><b>Oct 29th TENTATIVE:</b> (evening) EXAM 2</p> <p>(includes up to Diatomic Molecules)</p> |                                                   |
| Nov 3-5-10                                                                                    | <a href="#">Polyatomic molecules</a>              |
| Nov 12-17                                                                                     | <a href="#">Spectroscopy: Diatomics (Vib-Rot)</a> |
| Nov 19                                                                                        | <a href="#">Electronic Spectra</a>                |
| Nov 24 <sup>th</sup>                                                                          | <a href="#">Magnetic Resonance Spectra</a>        |
| Dec 1                                                                                         | <a href="#">EPR</a>                               |
|                                                                                               |                                                   |
| <p><b>Dec 8<sup>th</sup> TENTATIVE:</b> (evening) EXAM 3</p> <p>(includes up to EPR)</p>      |                                                   |