CHM 6470: Chemical Bond and Spectra

This class focus on fundamental concepts of quantum chemistry with applications to spectroscopy

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

Teaching Assistant: Vinicius Cruzeiro

CLASS SCHEDULE: Fall Semester 2014: August 22 – December 9. T, R Period 8-9 (3:00 pm-5:00 pm) @ CLB 313

No class on Nov 24 (thanksgiving).

OFFICE HOURS: Prof Kleiman: I have an open doors policy, so you can stop by my office (CLB 311B) at any time to see if I'm available. otherwise, send me an e-mail for an appointment.

T.A. Vinicius Cruzeiro (it WILL be changed after the 1week of classes): W 8th period (3:00-3:50 pm) Lei 442

TEXTBOOK: The material we cover is available on any Quantum Chemistry textbook for graduate level students. I will provide notes through the class web site (CANVAS). You can use the notes to see the topics we cover and go to ANY graduate level book for more "in-depth" reading. From time to time I will provide some additional reading too.

List of Possible Books

Molecular Quantum Mechanics by P.W.Atkins and R.S. Friedman

Quantum Chemistry by Ira N. Levine

Elements of Quantum Mechanics by M. Fayer

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. In addition to the 4 hrs class a week, ~8-10/week of reading, homework and general study are required.

COURSE SITE: We have a course workspace (http://lss.at.ufl.edu). 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 must be done professionally and formatted for presentation in an ACS journal. You will learn to use iPython, thus it is the first choice to use, but you can also use Matlab (free in UF comp. labs and as an App), 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.

During the course of the class we will introduce iPyhton as a resource for calculations and graphs.

EXAMS: There will be 2 progress exams. Conflicts with these exams dates (travel to conferences) 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.

COURSE GRADING: The grade will be determined by homework (25%), progress tests (35%), final project (30%) and in-class participation (10%).

There is NO FINAL in this class.

*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.*

Information on current UF grading policies for assigning grade points is available at https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx

COURSE EVALUATIONS Students are expected to provide feedback on the quality of instruction in this course by completing online evaluations at https://evaluations.ufl.edu. Evaluations are typically open during the last two or three weeks of the semester, but students will be given specific times when they are open. Summary results of these assessments are available to students at https://evaluations.ufl.edu/results/."

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 Classes

CHM 6470 FALL 2016

August

Tuesday	Thursday
23 Introduction to Ipython (Vinicius)	**25** Mathemathical Review: Differential equations. Homogenoues, inhomogeneous, Boundary Conditions (Levine Chp 2 pg 23-24). Diff equation of a wave. Its solutions (euler equation). Superposition of waves. Standing waves.
30 Introduction to Ipython (Vinicius)	

September

Tuesday	Thursday
	1 Matrices, eigenvalues and eigenvectors (Levine Molec Spec. Chp 2) Operators (Chp 3 Levine Quantum CHEM)
6 Dirac Notation. Opeartors, Commutators, Stern-Gerlach Experiment (app) Quantum Behavior/Wave Particle duality (ppt)	**8** Uncertainaty Principle. Born Interpretation. Free particles, Localization of wavepackets.
13 Schroedinger and Heisenberg Representations Particle in a box	**15** Particle in a box
20 Harmonic Oscilator	**22** Harmonic Oscilator (ladder operators)
27 Rigid Rotors (ring and sphere)	**29** Angular Momentum (with algebra of Operators)

October

Tuesday	Thursday
4 The H atom (SOLVING THE DIFFERENTIAL EQUATION)	**6** 2-state coupled system Spin and Coupling of angular momenta
11 Spin and Coupling of angular momenta	**13** Approximation Methods: Variational Theorem

18 Approximation Methods: Perturbation Theory	**20** Approximation Methods: Perturbation Theory
25 Time dependent Perturbation Theory: Spectroscopy	**27** Hartree-Fock Self Consisten Field

November

Tuesday	Thursday
1 Abinitio methods and DFT	**3** Diatomic Molecules
8 Diatomic Molecules/Semiempirical (Huckel)	**10** Semiempirical (Huckel)
15 GROUP THEORY	**17** GROUP THEORY
22	**24** **THANKSGIVING**
29 Project Presentation	

December

Tuesday	Thursday
	1 Project Presentation
6 Project Presentation	**8** **READING DAY**