Chemical Bond and Spectra

Course Information

Course number: CHM 6470
Course title: Chemical Bond and Spectra I
Credits: 3
Where: Room FLI 0109
When: Tuesdays and Thursdays; Period 7-8 (1:55 pm – 3:50pm)
No class on Nov 28^{th} (Thanksgiving)
List of Recommended Textbooks:
Molecular Quantum Mechanics by P.W.Atkins and R.S. Friedman
Quantum Chemistry by Ira N. Levine
Elements of Quantum Mechanics by M. Fayer

Online material: Available through canvas (https://elearning.ufl.edu/)
It will contain the syllabus, howework and lecture notes. It will also serve as a mode of email communication (you can configure it to redirect the emails).

Instructor Information

Alberto Perez
Assistant Professor
Office: Room 240F Leigh Hall.
Office hours: By appointment.
Contact e-mail: perez@chem.ufl.edu

Homework and Grading

Attendance: Attendance to lectures is expected. The 2-period class will combine a traditional lecture with discussion of problems as time allows. In addition to the 4 hrs class a week, ~8-10/week of reading, homework and general study are required.

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.

Python notebooks: When possible, we'll try to use python notebooks for homework and graphics. This provides a great environment for paper publication ready figures as well as a great environment to handle data.

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.

Final Projects: Consist of two parts. More details will be forthcoming during the year.
1. A python script or python notebook for running a Huckel or Extended Huckel calculation. This can be done in groups.
2. An end of year TED-like formatted talk to make QM topics more accessible to the general public.

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.

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.
On all work submitted for credit by students at the university, the following pledge is either required or implied: On my honor, I have neither given nor received unauthorized aid in doing this assignment.

Cheating on an exam will result in a grade of zero. Although homework is 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

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.

Course Objectives

By the end of this course students should be able to:

1. Understand the need of a mathematical formalism to describe the behavior of atoms and molecules: quantum chemistry
2. Describe the meaning of the wavefunction as it relates to atoms and molecules
3. Apply their knowledge on quantum chemistry and wavefunctions to solve the Schroedinger equation for simple cases (e.g. harmonic oscillator)
4. Explain and apply approximate methods (variation method and perturbation theory) to solve more complex cases (e.g. polyatomic molecules)
5. Relate the mathematical knowledge and applications to experimental observables (e.g. spectroscopic signals)

Course itinerary:

- **Working with python notebooks**
- **Mathematical review**: Differential equations, complex numbers, matrices, waves, eigenvalues/eigenvectors, operators, Dirac Notation.
- **Quantum behavior**

TENTATIVE Schedule of Classes

CHM 6470 FALL 2016

August	
Tuesday	**Thursday**
20 Introduction to the course	**22** Mathemathical Review: Differential equations. Waves
27 Superposition of waves. Standing waves. Matrices	**29** Matrices, eigenvalues and eigenvectors (Levine Molec Spec. Chp 2)

September

Tuesday	Thursday
3 Operators (Chp 3 Levine Quantum CHEM)	**5** Dirac Notation. Operators, Commutators, Stern-Gerlach Experiment (app) Quantum Behavior/Wave Particle duality (ppt)
10 Uncertainaty Principle. Born Interpretation. Free particles, Localization of wavepackets.	**12** Schrodinger and Heisenberg Representations Particle in a box
17 Particle in a box (infinite, finite)	**19** 1-D 2-D finite potentials
24 Harmonic Oscillator (ladder operators)	**26** Harmonic oscillator functions, graphics, calculation of observables . Ang. Mometum

October

Tuesday	Thursday
1 Angular Momentum (with algebra of Operators) Particle in a RING	**3** Rigid Rotors. Schroedinger equation, separation of variables, Functions, degeneracy, Solutions (gral and in particular)
8 The H atom (SOLVING THE DIFFERENTIAL EQUATION)	**10** H-atom: THE SOLUTIONS SPIN
15 2-state coupled system Coupling of angular momenta	**17** Approximation Methods: Variational Theorem
22 Approximation Methods: Perturbation Theory	**24** Approximation Methods: Perturbation Theory
29 Time dependent Perturbation Theory: Spectroscopy	**31** Hartree-Fock Self Consistent Field

November

Tuesday	Thursday
5 Ab-initio methods and DFT	**7** Diatomic Molecules
12 Diatomic Molecules/Semiempirical (Huckel)	**14** Semiempirical (Huckel)

19 GROUP THEORY	21 GROUP THEORY (spectroscopy)
26 Course recap	28 Thanksgiving, No classs

December

Tuesday	Thursday
3 Project presentation	5 Project presentation
10	12