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 8-9 (3:00 pm – 4:55pm)
No class on Nov 24 (Thanksgiving)
Recommended Textbook: Quantum Chemistry by Ira N. Levine. 6th edition
Online material: Available through canvas (https://elearning.ufl.edu/)
It will contain the syllabus, homework and lecture notes. It will also serve as a mode of email communication (you can configure it to redirect the emails).

Instructor Information

Name: Alberto Perez
Title: Assistant Professor
Temporary office: Room 354 Leigh Hall.
Office hours: I have an open doors policy. If you drop by and I'm not available you can send me an email for an 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 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.

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.

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.
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 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.

Students Requiring Accommodations

Students with disabilities requesting accommodations should first register with the Disability Resource Center (352-392-8565, www.dso.ufl.edu/drc/) by providing appropriate documentation. Once registered, students will receive an accommodation letter which must be presented to the instructor when requesting accommodation. Students with disabilities should follow this procedure as early as possible in the semester.

Class Demeanor

Students are expected to arrive to class on time and behave in a manner that is respectful to the instructor and to fellow students. Please avoid the use of cell phones and restrict eating to outside of the classroom. Opinions held by other students should be respected in discussion, and conversations that do not contribute to the discussion should be held at minimum, if at all.

Counseling and Wellness Center

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

The course aims at an understanding of the basic principles of Quantum Chemistry. By the end of the course students should be able to:

1. Understand the need of a 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 Schrödinger equation for simple cases (e.g. harmonic oscillator)
4. Describe and apply approximate methods (variation method and perturbation theory) to solve more complex cases (e.g. polyatomic molecules)
5. Relate the formalism studied to applications in Chemistry

Course itinerary:

The following itinerary is tentative.

Week 1: Intro to the course and python notebooks.

HW0: Introduce yourselves on Canvas.

Week 2: Mathematical review: Differential equations. Homogenoues, inhomogeneous, Boundary Conditions (Levine Chp 2). Differential equation of a wave. Its solutions (euler equation).Superposition of waves. Standing waves.

HW 1

Week 3: Mathematical review: Matrices, eigenvectors and eigenvalues. Operators (Chapter 3 Levine)

Week 4: Dirac Notation, Quantum Behavior, wave/particle duality. Uncertainty principle. Free particles

HW2

Week 5: Schrödinger and Heiseberg representations. Particle in a box

HW3

Week 6: 1D, 2D finite potentials. Harmonic Oscillator

Week 7: Harmonic Oscillator functions, graphics. Angular momentum

HW4

Week 8: Rigid Rotors, Schrödinger equation. Functions, degeneracy, solutions.

Week 9: The H-atom. Spin

Exam 1

Week 10: 2 –state coupled system. Coupling of angular momentum. Variational theorem

Week 11: Perturbation theory

HW5

Week 12: Time-dependent perturbation theory: Spectroscopy.

HW6

Week 13: Hartree-Fock Self Consistent field

Week 14: Ab initio methods and DFT

HW7

Week 15: Diatomic Molecules

HW8

Week 16: Diatomic Molecules/ Semiempirical (Hückel)

Week 17: Group theory

Exam 2

Week 18: Presentation of projects