CHM 6490 MOLECULAR SPECTROSCOPY
Spring Semester 2015

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

CLASS SCHEDULE: January 6th – April 21st
Tuesdays 9:30 – 11:30 am and Thursdays 9:30 – 10:30 am@ CLB 313
Office hours by appointment.

PREREQUISITES: The course requires a graduate level Quantum Mechanics course as prerequisite. Mathematical background substantially beyond proficiency with matrix representations and linear algebra should not be necessary. Along with traditional methods for analyzing spectra, I will show a time dependent approach to interpretation of molecular spectra and introduce also modern spectroscopic methods. The theoretical framework presented in this course is common to most modern spectroscopies (including electronic, vibrational and nuclear methods). Numerical methods to simulate spectra will be introduced in homework assignments.

TEXTBOOK: Some (but not all) of the class will cover topics presented in J. L. **McHale – Molecular Spectroscopy** (Prentice Hall, 1999). This is the primary text. It is very readable and intuitive but not always completely rigorous. (You get extra points for finding errors in equations in the text☺).
G. C. Schatz and M. A. Ratner – Quantum mechanics in chemistry, (Prentice Hall, 1993). This book provides in Chapter 9 an introduction to the time-dependent approach to spectroscopy.

In addition, we'll make extensive use of lecture notes.

TOPICS
-   Review of QM simplest models and approximation methods
-   Maxwell Equations
-   Time dependent Quantum Mechanics
-   Schrödinger, Heisenberg Representations and Interaction Picture
-   Propagators for time dependent and time independent Hamiltonians
-   Time dependent Perturbation Theory (1st and higher orders)
-   Solutions for Time-dependent Perturbation (harmonic oscillators, Irreversible relaxation, Step Function, Adiabatic perturbations)
-   Fermi Golden Rule
-   Light-Matter interactions (classical)
-   Einstein Coefficients, Spontaneous emission
-   Symmetry, Molecular transitions and selection Rules
-   Review of Statistical Mechanics, Density Matrix description
-   Time Correlation Functions
-   Absorption Lineshapes for Rotations, Vibrations, Ramman
-   Inhomogeneous and Homogeneous Broadening (lineshapes)

HOMEWORK & ASSIGNMENTS: The class will have a combination of homework and project assignments. This is a graduate course and the expectation is that you'll learn to study and to work independently. As a PhD student, and for the rest of your scientific career, you will do experiments for which the answers are not known. ***It is critical that you learn to assess the correctness of your results on your own.*** How do you do that? You compare to previous work, establish a correct method, check for similar problems, compare with the work of others and test your results. In this course we will attempt a step on this direction by working on homework assignments for which answers will not be provided. I'll be available to consult and help with any homework problem, but only to guide you through the process.

The assignments will include a small amount of programming.

COURSE GRADING: The grade will be determined by progress tests, in-class participation and a final project.

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.