CHM4412:
Quantum Mechanics and Spectroscopy

Fall 2019 4 credit hours

Class Number(section): 11560(0823)

T R Periods 7-8 (13:55 - 15:50) LEI207

No (specifically) Required Textbook:
Useful texts include *the one you have* or something like:
Physical Chemistry, P. W. Atkins *et. al.*,
or similar titles by McQuarrie & Simon, Levine, Raff, Castellan
Complete notes for this course will be provided (free), but this subject is enriched by multiple perspectives and interpretations, so you should have your own physical [*sic*] textbook(s) for breadth of understanding.
See Brucat if you have questions...

Instructor: PJ Brucat
- Office location: CLB311
- Scheduled (group) office hours (subject to change):
  Tuesday's Periods 3-4 (09:35 - 11:30)
  Thursday's Periods 4-6 (10:40 - 13:40)
- Private office hours:
  by Appointment, offer three choices (see below)
- Contact method: *Canvas Messaging only*

TA: Arup Mondal

Course Website:
https://ufl.instructure.com/courses/376517/
All course materials and course communications, will be delivered from within UFs eLearning system (Canvas) at the URL above. Please become familiar with our course website as soon as possible. Note that the materials there will be subject to change, so pay attention to all announcements and publication dates. It is strongly suggested that printing or static downloads be avoided.

Course Goals

Successful completion of this course will increase and refine knowledge and proficiency in these areas:
- The Scientific Method
- The Postulates/Assumptions/Tenants of Quantum Mechanics
- Methodology for the Mathematical Description of Quantum Mechanical Systems
- Computational Methods for Symbolic and Numerical Mathematics and Data Analysis
- Uniquely Quantal Phenomena such as Uncertainty, Entanglement, and Observer Interaction
- Fundamental Properties of Chemical Bonds and Bonding
- The Mathematics of Symmetry and its Application to Chemistry
- Spectroscopy of Atoms and Molecules

Course Objectives
Mastery of the course material will be assessed in the following topics:

- Knowledge
  - Guiding Principles in Mechanics
  - Operators, Wave Functions, and the Schrödinger's Equation
  - Eigenstates, Uncertainty, and the Act of Measurement
  - Time Dependence and Superposition of Quantal Systems
  - Representations and Operator Algebra
  - Approximate Methods in Quantum Mechanics
  - Properties of Simple Systems (PiB, SHO, Hydrogen Atom, Hydrogen Molecule, *etc.*)
  - Classification and Consequences of Molecular Symmetrya
  - The Hierarchical and Quasi-Separable Nature of Molecular Motion
  - Models Used in the Description of Chemical Bonding
  - Semiclassical Interaction of Light with Matter
  - Fundamentals of Common Spectroscopic Methods (UV-Vis, IR/Raman, $\mu\lambda$, NMR, *etc.*)
  - Non-Linear and Coherent Methods in Modern Spectroscopy
- Skills
  - Use of Computational Tools in the Solution of Complex Mathematical Problems
  - The Generation of a Quantum Mechanical Equation of Motion for an Arbitrary Atomic or Molecular System
  - Apply Differential Equation Methods to the Solution of Quantum Mechanical Problems
  - Apply Linear And Operator Algebra to the Solution of Quantum Chemical problems
  - Identify and Apply Appropriate Approximate Methods to Quantum Mechanical Problems
  - Apply Group Theoretical Methods to Simplify Quantum Mechanical Problems
  - Analyze and Interpret Molecular Spectra for the Purpose of Extracting Chemical Information
  - Interpret the Mathematical Results of a Quantum Calculation in Terms of a Picture of the Universe

Mediasite: All lectures will be recorded and posted in a Mediasite Catalog
Communication with your Instructor All course communications with your Instructor(s) are to occur within the Canvas environment using the embedded tools. Configure your Canvas account profile now for immediate automatic notification of course announcements and updates. Responsibility for receiving and responding to electronic course communication in a timely fashion is entirely that of the student.
Scheduled Office Hours and Meetings by Appointment Scheduled office hours held by Brucat are intended for discussion of corse content and are available to everyone on a walk-in basis. Meetings by appointment are intended for one-on-one discussion of a students standing in the class (grades), learning strategy and habits, remediation of specific hindrances to individual learning, and any other things not appropriate for group/public discussion. These private discussions will be held at times you arrange, subject to Instructor availability. If you want a private meeting of this sort, message your Instructor (from within Canvas, only) 3 options for meeting times, and your Instructor will reply with a choice that works best and a location for the meeting.
Attendance Your prompt attendance at all our scheduled class times is *required*. If you are unable to make a class for some reason, please message the Instructor (within Canvas) *before* the scheduled class time. Excused absences are defined by University attendance policy. Unexcused absences will result in grade penalties at the discretion of the Instructor.
Etiquette Your polite, courteous, and civilized behavior is expected in all aspects of our course. This holds especially true for electronic and interpersonal communication with your peers and your Instructor.

Course Operation The structure of the course consists of physical meetings twice a week in a classroom. Some of this time will be used in the traditional lecture method of teaching, some group discussion, and some learners working problems on the board with the remainder of the class participating in support. Research has shown that lectures are most effective when they are prepared for, absorbed, and reviewed/discussed (three steps). Then, exercises will challenge your understanding through problem solving, These exercises will consist of three types: Concept Quizzed (trivial), ClassWork (involved asynchronous), and Exams (mastery assessment).

Course Activity Types

Lecture Preparation Before every class meeting, a preparation assignment will be posted. At the very least it will include some reading, and also a look at relevant problems (CourseWork or CW, see below) that will be submitted after the lecture is given. Lecture preparation Assignments are not graded.

Live Lecture/Discussion Twice a week, we will meet for two hours to discuss Quantum Mechanics, Specroscopy, and Chemistry. The Discussion will be lead by Brucat, based on the course notes, but will be guided by your questions and comments. These lectures will be recorded *vide supra*

Lecture Review After each lecture, there will be a Community Review assignment delivered in VoiceThread. The assignment will typically be to post comments on the lecture nottes displayed, but other activities may be requested. Read the assignment instructions for details.

Concept Quizzes (CQ) Periodically throughout the term, short/trivial question sets will be delivered online through our course website. Thorugh Lecture Preparation and Review should make these enjoyable and quick.

Course Work (CW) Traditional classes have you, the student, work exemplary problems to cement your mastery. These are often worked outside of class, usually alone. We are going to work those problems in class, together. A portion of your grade will be derived from these problem sessions, so be prepared.

Exams There will be four in-class exams during the term. These are typically 5-6 page white-space closed-book tests, with a page or two of given information (fact sheet) to assist your work. These Exams will be graded and reviewed in class by your instructor.

All activity dates and grades are posted on the course website in Canvas. Assignments are to be submitted in full by the assignment deadline for credit.

Course Resources and Ancillary Materials

- Course Content and Materials
  - Lecture Notes
    All of Brucat's lecture notes will be posted on the Canvas course website before the material is discussed in our class meetings. Direct link to these notes will be available in the Lecture Preparation assignment (0 grade points) associated with each lecture. You are expected to read the lecture notes prior to attending the lecture, identify where in your textbook this material resides, and read that material as well to provide context and background. The entire course notes will be available in a "book" format by the end of the term for future reference.
  - Lecture Video Recordings
    All live lectures will be recorded in the classroom and available through UF's Mediasite Catalog.
  - Lecture Review/Discussion (VoiceThread)
    After each lecture, a Lecture Review Assignment (10 grade points each, total = 10% of the course grade) will be posted. These assignments are delivered through VoiceThread, and are populated with the lecture slides. You will be asked to comment and discuss the content of the lecture and the comments of you peers. Comments will be graded as following the guidelines of the assignment (full credit) or not (0 credit). All lectures will have a corresponding review assignment. Access the Lecture Review through the Canvas Assignment link *only* and submit your comments using the green submit button. Comments not submitted will not generate grade points.
- Computational Mathematics Tools
  - UF Apps (Useful if all else fails)
    UF students have a powerful suite of software tools available to them via the UF Apps web (Citrix) interface. Included in these "apps" are some quite sophisticated tools to assist in the symbolic and numerical solution to mathematical problems as well as the visualization of these results. A few that should be familiar are *Mathematica* (The best IMHO), Maple, MatLAB, R, SAS, SPSS, among others. Some of these packages are great, but quite expensive (*Mathematica*!) so your access for life is not guaranteed.
  - iPython/Anaconda/Jupyter
    One of the most active and interesting platforms for computation is interactive Python as delivered through a cell-based "notebook". This environment resembles some of the features of the *Mathematica* app, but has two advantages: It is community-supported an open source (free!), and it is becoming a standard for use by Chemical researchers, data scientists, and many other smart people. This means familiarity with Python may just get you a job, or be in your career path whether you like it or not. For that reason, I have switched from *Mathematica* to Python for my work (YMMV). So, how does one get started with iPython notebooks? Two choices:
    1. **Install "Anaconda" on your own device** (Recommended for general utility) "Anaconda" is a code suite that allows one to easily setup Jupyter/iPython/R on your own device. If you are in possession of a laptop or desktop and do any sorts of analysis with it, you should have Anaconda at your disposal. The free download and instructions can be found on the website: https://www.anaconda.com/distribution/. Anaconda is also available through UF apps, which may be useful once you become a Python expert.

2. **Use the Chemistry Jupyter Server** (Recommended for graded assignments in this course) A ready-to-go, web-accessible Jupyter server has been created for use in this course. If you put your work their, the instructor can look at it immediately when questions arise and provide tips and hints right in your notebook. The server can be found here: https://jupyter.chem.ufl.edu:8000/. Login there with your Gatorlink username (the part of your @ufl.edu email address before the @ symbol) and the initial password "mechanicup". Instructions for changing your password to protect your work will be provided. If off campus, VPN into the UF network first.

- Quantum Chemical Calculation Tools (WebMO)
  There are several sophisticated software packages available for the computation of the electronic structure of isolated molecules. These tools are extremely useful in testing and learning the concepts of Quantum Mechanics in their application to Chemistry. A few of the most powerful tools have been aggregated and access provided to you through a web interface called "WebMO". The login is here: http://webmo.chem.ufl.edu/~webmo/cgi-bin/webmo/login.cgi Login with your GatorLink username (the part of your @ufl.edu email address before the @ symbol) with the initial password "mechanicup" (without the quotes). Change your password immediately ("Utilities" ⇒ "Edit Profile") to protect your work. If off campus, VPN into the UF network first. The use of this tool will be discussed at the appropriate time in the semester, but feel free to wade around if you feel like it.

Learning Quantum Mechanics is Personally Challenging

A little over a 100 years ago, no human actually fundamentally understood the nature of matter, or light, or how they interact. Yet, up to that point in history, humans were really pretty good at manipulating light and matter, and Chemistry as a discipline was fairly well established and powerful, all by the brute force of the scientific method fueled by the insatiable need to control and manipulate of the environment in which we live.

At the turn of the 20^{th} century, human ignorance was confronted with a strange and inevitable consequence of inexplicable observations, which gave rise to new ideas, a set of which is called Quantum Theory. These ideas lead to an exponential growth in Science, and most importantly Chemistry. The predictions of this Quantum Theory are testable, and have proven to be robust. However, the interpretation of the quantum world is still in debate to this day.

To a certain extent interpretation is a problem in Philosophy, not Chemistry, and therefore somewhat moot. However, to a student of Quantum Mechanics, such interpretation(s) are important, if not crucial, to the learning process. But, unlike many other fields, these interpretations have a tendency to change as understanding matures. What is immutable, however, is the *process* by which we approach the development of Quantum Mechanics, or any theory: We make some assumptions, we employ irrefutable logic (Mathematics) to those assumptions to make predictions, and test those predictions with experiment. If all goes well, a discord is found between the predictions and the truth, and something is learned (new assumptions are needed). If the boring agreement between predictions and observation results, we try to make make a bolder prediction until something breaks. This is the scientific method: Learning by Breaking Things.

Experiments will not be performed first hand in this class, but experimental results from human history and your associated laboratory courses will be brought to bear. We will explore the path from assumptions to predictions in much the same way the ancients did (but with fewer missteps) and try to develop interpretations of these predictions that we *as individuals* believe. Your interpretation of Quantum Mechanics may be different than mine, which is perfectly fine, as long as accurate predictions are made from our respective philosophies. The important thing to remember is one has to develop *their own* interpretation of the microscopic world which cannot be gifted or copied (sadly).

For each student to be able to make their own interpretation of Quantum behavior, the path between assumption and perdition must be understood. That means Math. Some of this Math may not be familiar to you, and some of it is just plain cumbersome. Unlike the ancients, we have tools to help us with the Math that will lead us to enlightenment without needless toil. These tools will be integrated [*sic*] into our discussions and are valuable not just for this study, but for problem solving and data analysis of all types. You may find that the exercises in symbolic and numerical computation performed in this course of study are some of the most valuable and long lasting benefits of of your efforts.

Course Grade Computation: Course grades will be computed from the weighted-average of the earned percentages of each graded item submitted by the student. The weighting factors are as follows:

Category Weights

Grade Category	weight %
Lec Prep	0
Lec Review	10
Quiz (CQ)	10
CourseWork	10
Exams	70

Grade Percentages

Grade	A	A−	B+	B	B−	C+	C	D	E
Minimum percentage	87.5	80.0	77.5	72.5	70.0	67.5	60.0	50.0	< 50.0

Regrade Requests Assignments will be regraded if an error is suspected. Regrade requests must be submitted through Canvas Messaging within 72 hours of the grade post. Regrades will be performed on the entire assignment.

UF's Grading Policy: See http://www.registrar.ufl.edu/grades/gradepolicy.html and https://catalog.ufl.edu/ugrad/current/regulations/info/grades.aspx

Honesty and Truthfullness: Ethical, moral, and professional behavior is expected and required of all participants in this course. Moreover, all participants in UF's Academic activities are bound by Rules of Conduct, from which can be found:
"UF students are bound by The Honor Pledge which states,
'We, the members of the University of Florida community, pledge to hold ourselves and our peers to the highest standards of honor and integrity by abiding by the Honor Code.'
On all work submitted for credit by students at the University of Florida, the following pledge is either required or implied:
'On my honor, I have neither given nor received unauthorized aid in doing this assignment'
The Honor Code (http://www.dso.ufl.edu/sccr/process/student-conduct-honor-code/) specifies a number of behaviors that are in violation of this code and the possible sanctions. Furthermore, you are obligated to report any condition that facilitates academic misconduct to appropriate personnel. If you have any questions or concerns, please consult with the instructor or TAs in this class"

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.

Counseling: Useful non-academic services are available in many forms at UF. A good source of information is the Counseling and Wellness Center: http://www.counseling.ufl.edu/cwc/

GatorEvals: "Students are expected to provide professional and respectful feedback on the quality of instruction in this course by completing course evaluations online via GatorEvals. Guidance on how to give feedback in a professional and respectful manner is available at https://gatorevals.aa.ufl.edu/students/. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals, in their Canvas course menu under GatorEvals, or via https://ufl.bluera.com/ufl/. Summaries of course evaluation results are available to students at https://gatorevals.aa.ufl.edu/public-results/."

All course policies and procedures are subject to change at any time at the sole discretion of Brucat

We, the members of the University of Florida Community, pledge to hold ourselves and our peers to the highest standards of honesty and integrity

— PJ Brucat 08/19/2019 —