CH 4412 - Quantum Mechanics and Spectroscopy

Instructor: Prof. John F. Stanton (NPB 2336, johnstanton@ufl.edu) Office Hours: TBA

Teaching Assistants: Rohit Rana and Josie Kilburn

Office Hours: TBA

Textbook: None

Week	Dates	Material
Fundamental Quantum Mechanics		
Ι	Jan $12^{\dagger}, 14$	Boot Camp
II	Jan 19,21	Boot Camp and Historical Background
III	Jan $26^{\dagger \ddagger}, 28$	Postulates of Quantum Mechanics
IV	Feb $2,4$	Solvable Problems I
V	Feb $9^{\dagger \ddagger}, 11^{*}$	Solvable Problems II
VI	Feb 16,18	Solvable Problems III
VII	Feb $23^{\dagger\ddagger}, 25$	Solvable Problems IV
Applications of Quantum Mechanics		
VIII	Mar 2,4	Application of Approximate Methods to Simple Problems
IX	Mar $9^{\dagger \ddagger}, 11^*$	The Hydrogen and Helium Atoms
Х	Mar 16,18	Hartree-Fock Theory and Orbitals
XI	Mar $23^{\dagger\ddagger}, 25$	What is a Molecule? The Born-Oppenheimer Model
XII	Mar 30, Apr 1	Diatomic Molecules I
XIII	Apr $6^{\dagger\ddagger},\!8^*$	Diatomic Molecules II
XIV	Apr 13,15	Polyatomic Molecules
XV	Apr 20 [‡]	Wrapping Up

Course Schedule

† - Homework assignments will be passed out.

‡ - Homework assignments will be collected.

* - Hour examination will be administered.

Class Website

The class website is hosted on piazza, from which you have obtained this syllabus. In addition to posting notes, homework and exam solutions, and so on, piazza is also an extrememly useful resource for asking questions outside of class and/or office hours. This system has been quite effective and popular since I started to use it a several years ago, and <u>you</u> are encouraged to answer the questions of your classmates if you are able. The TAs and I will also answer questions in a time frame ranging from "right away" to a few days, but all of you are encouraged to help each other and post answers if you think that they are correct. Both the TAs and I will monitor the goings on, and will intercede with corrections when and if warranted.

Scope of Material

CHM 4412 covers the subject of quantum mechanics from a chemist's point of view. The course will begin with a "review" of concepts from mathematics (trigonometry and calculus, primarily) that are seen again and again in this course, followed by a historical overview of the subject, covering physics from the time of Newton to the dawn of a new age at the beginning of the 20th century. This is followed by an outline of the framework of quantum mechanics and its application to model systems for which the Schrödinger equation can be solved exactly. In chemistry, however, *all* systems of interest involve mathematically intractable Schrödinger equations and approximations are the name of the game. The rest of the course deals with the fundamental principles that underlie atoms and molecules: the existence of discrete energy levels, their qualitative interpretation, and the ability of electromagnetic radiation (photons) to induce transitions between these levels, and some connections between quantum mechanics and thermodynamics. I will warn you now that this course (particularly the early part of it) involves some rather serious and involved mathematics. If you were overwhelmed with the math encountered in CHM 4411, you might find yourself significantly more overwhelmed by this course. It's tough, but worth it for those who expend the effort.

Homework

Homework problems will be assigned every other Tuesday throughout the semester and are due at the beginning of class two weeks later. Assignments turned in later than 3:05 PM on the specified Tuesday will not be accepted. If you anticipate that it will be impossible to arrive by that time, there are three options: 1) get a friend to turn it in for you; 2) slide your homework under my office door sometime BEFORE 3:00 PM on Tuesday afternoon; 3) make arrangements with a TA to send it to them electronically sometime before the deadline. Please show all work on the sheets provided in the homework packet. If there is not enough room underneath the problem statement to write down your calculations and/or reasoning along with the solution, you should attach extra pages to the assignment packet, order them properly and then restaple it before submission. For those of you who want challenging and sometimes algebraically brutal problems, I will not disappoint. For the most part, homework assignment is due in class. As an example, the problems assigned on the Tuesday of Week V will be due in class on the Tuesday of Week VII, and will mostly cover material from Weeks V and VI. Solution sets will be posted on piazza, usually on the evening after the homework is due.

Examinations

There will be three open-book, open-note examinations administered during the usual class time, as well as a final examination. I expect you to be responsible and avoid scheduling conflicts that interfere with exams. Take note of the exam dates *now* and plan things such as medical school interviews accordingly. I rarely give make-up exams, and generally do so only for very good reasons (medical and family emergencies, religious holidays *etc.*).

Grading Policy

The basis for grades in CHM 4412 will be performance on the hour exams, the final exam and the homework assignments. Only the five highest of seven homework scores will be counted. The distribution of points is given below.

200
200
200
200
200
1000

In general, the basis for grade assignment is the class score distribution; those of you scoring above roughly the median will receive an A or B; those scoring below generally receive a C, D or F. However, who score above 850 are guaranteed an A, while those scoring above 700 are guaranteed at least a B grade. While I generally do not give a lot of A's, it works both ways: only truly determined students who dedicate themselves to not trying or working hard will get a D or a failing grade.

Advanced Warning: You should not take this class unless you are ready to do a fair amount of work. While I previously thought "senioritis" was a disease that afflicted only high school students, there seem always to be a few students in 4412 that suffer from it. If you make an effort, you are certain to pass the class, but you do need to make an effort.

COVID-19 Considerations

While you have the good fortune to benefit from face-to-face instruction, it remains true that education during a pandemic will not conform to normalcy. Accordingly, you must obey the masking and social distance rules of the University of Florida (see this link) during classroom sessions. That is, 1) you are permitted to sit *only* in the seats explicitly reserved within Flint 0050; and 2) you must wear a mask (covering your nose and mouth at all times) during class and elsewhere within Flint Hall. Anyone who does not follow these mandates in the classroom will be asked to leave, and will face potential disciplinary action from the university. It will be a weird experience – I will lecture from behind a mask, and you will sit, take notes, and ask questions from behind your own masks – but ultimately I am confident that it will be vastly superior to a "zoom class". Let's follow the rules, stay safe, and look towards a brighter future.

Disabilities

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

Counseling

The University of Florida provides counseling services for students, staff, and faculty. See this link or call (352) 392-1575 during regular service hours (8am 5pm). For other hours or on 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.

Honor Code

This class will operate under the policies of the student honor code, which can be found here. 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.

Evaluations

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 here. Students will be notified when the evaluation period opens, and can complete evaluations through the email they receive from GatorEvals. Summaries of course evaluation results are available to students here.