

CHM 4412: Quantum Mechanics and Spectroscopy

Term: Fall 2020

Instructor: Ramón Alain Miranda Quintana

Teaching assistant: Liwei Chang

Office: Leigh Hall, 240H

Phone: 352 294 3489

Email: quintana@chem.ufl.edu

Class schedule: T,R | Period 7 - 8 (1:55 PM - 3:50 PM)

Office hours: Since all our interactions are anticipated to be online office hours won't follow the standard patterns. I'll leave Fridays 1-3 pm free so if you want to meet we can schedule a Zoom meeting (individually or in groups). If you want to meet at other day/time please send me a message and we can arrange other sessions.

Prerequisites: This class makes extensive use of mathematics (integration, differentiation, algebra, complex numbers, trigonometric functions, etc.). If you are not up to speed in your math skills, you need to work on that in the first week of the semester. I'll refresh some math concepts and "tricks" during the lectures, and we'll practice the necessary math skills in the homework assignments along the course. Be sure you feel comfortable with these concepts so you can concentrate on the physical chemistry.

Books: The material we cover is available on any Quantum Chemistry textbook for undergraduate level students. I will also share notes and materials that will complement the more "traditional" topics with some new concepts and ideas. A list of recommended books includes:

Physical Chemistry, a Molecular Approach by D. McQuarrie.

Physical Chemistry by P. Atkins.

If you are interested in more advance topics (graduate level), **Quantum Chemistry** (Ira N. Levine) is an excellent book.

Course objective and goals:

This course will give cover quantum mechanics and spectroscopy from a chemist's point of view. A tentative list of topics that we will cover includes explaining why quantum mechanics can be seen as the basis of modern chemistry and physics, and the experiments/developments that led to the realization that we had to move on from a classical ("Newtonian") view of the Universe. We will discuss the postulates that serve as the basis for quantum mechanics, alternating between "analytical" and "algebraic" representations (Dirac notation) of quantum states and observables. We will introduce many concepts via the analysis of multiple systems (e.g., free particles, the rigid rotor, the harmonic oscillator, etc.) that can be solved exactly using elementary quantum mechanics' tools. Of particular importance will be the introduction of basic techniques (the variational principle and perturbation theory) used to solve more realistic problems, which we will apply to the study of model chemical systems. We will explore the quantum mechanical nature of atoms and molecules, with particular emphasis on the electronic (and, later on, nuclear) spin, potential energy surfaces, molecular symmetry, etc. We will introduce (at a basic level) several modern computational chemistry models that are routinely applied in the study of molecules and materials (Hartree-Fock, Configuration Interaction, Density Functional Theory, etc.). The last part of the course will be devoted to different spectroscopy techniques (UV, IR, NMR), we will mostly describe their foundations, but we will also present some simple applications.

Evaluations and grading:

We will have homework problems approximately every week. Homework due date will be announced in class and posted on the class calendar. Late homework will not be accepted. For most of the problems you will be asked to provide the full derivation, using SI units. It is expected that the students will collaborate on some of the problems but, unless otherwise indicated, the homework must be delivered individually. We will also have quizzes that will be posted shortly after some lectures.

There will be 3 progress exams. Conflicts with these exams dates (travel to conferences, visiting graduate schools) 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. There will be a (short) comprehensive final exam that will have the same weight as the 3 progress exams.

There will be no make-up exams.

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

The grades will be determined as:

Exams---40%

Homework----40%

Quizzes----10%

Class participation/engagement----10%

Letter grade	From	To
A	87	100
A-	84	86.99
B+	81	83.99
B	78	80.99
B-	75	77.99
C+	72	74.99
C	69	71.99
C-	66	68.99
D+	63	65.99
D	60	62.99
D-	50	59.99
E	0	49.99

More information on current UF grading policies for assigning grade points can be found at: [link to the university grades and grading policies](#).

Accommodations for students with disabilities: Students with disabilities who experience learning barriers and would like to request academic accommodations should connect with the disability Resource Center. [Click here to get started with the Disability Resource Center](#). It is important for students to share their accommodation letter with their

instructor and discuss their access needs, as early as possible in the semester.

Privacy related issues: Our class sessions may be audio visually recorded for students in the class to refer back and for enrolled students who are unable to attend live. Students who participate with their camera engaged or utilize a profile image are agreeing to have their video or image recorded. If you are unwilling to consent to have your profile or video image recorded, be sure to keep your camera off and do not use a profile image. Likewise, students who un-mute during class and participate orally are agreeing to have their voices recorded. If you are not willing to consent to have your voice recorded during class, you will need to keep your mute button activated and communicate exclusively using the "chat" feature, which allows students to type questions and comments live. The chat will not be recorded or shared. As in all courses, unauthorized recording and unauthorized sharing of recorded materials is prohibited.

Honor pledge: 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 specifies a number of behaviors that are in violation of this code and the possible sanctions. [Click here to read the Honor Code.](#) 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.

Campus

Resources:

Health and wellness:

U Matter, We Care: If you or someone you know is in distress, please contact umatter@ufl.edu, 352-392-1575, or visit [U Matter, We Care](#)

[website](#) to refer or report a concern and a team member will reach out to the student in distress.

Counseling and Wellness Center: [Visit the Counseling and Wellness Center website](#) or call 352-392-1575 for information on crisis services as well as non-crisis services.

Student Health Care Center: Call 352-392-1161 for 24/7 information to help you find the care you need, or [visit the Student Health Care Center website](#).

University Police Department: [Visit UF Police Department website](#) or call 352-392-1111 (or 9-1-1 for emergencies).

UF Health Shands Emergency Room / Trauma Center: For immediate medical care call 352-733-0111 or go to the emergency room at 1515 SW Archer Road, Gainesville, FL 32608; [Visit the UF Health Emergency Room and Trauma Center website](#).

Academic Resources:

E-learning technical support: Contact the [UF Computing Help Desk](#) at 352-392-4357 or via e-mail at helpdesk@ufl.edu.

Career Connections Center: Reitz Union Suite 1300, 352-392-1601. Career assistance and counseling services.

Library Support: Various ways to receive assistance with respect to using the libraries or finding resources.

[Teaching Center](#): Broward Hall, 352-392-2010 or to make an appointment 352- 392-6420. General study skills and tutoring.

[Writing Studio](#): 2215 Turlington Hall, 352-846-1138. Help brainstorming, formatting, and writing papers.

Student Complaints On-Campus: [Visit the Student Honor Code and Student Conduct Code webpage for more information.](#)

On-Line Students Complaints: [View the Distance Learning Student Complaint Process.](#)