

Chemical Bond and Spectra I – CHM 6470 Syllabus

CHM 6470, Fall 2022, Tuesday, Thursday, 9:35 am – 11:30 am

Room: FLI 0109. Lectures scheduled for synchronous delivery on Canvas

Instructor: Mingjie Liu, mliu@chem.ufl.edu, Office: LEI 240C;

Course Description. This class focus on fundamental concepts of quantum chemistry with applications to spectroscopy. The frontier research topics (e.g. high-performance computing and artificial intelligence) related to quantum chemistry will be introduced as well.

Course Coverage. Basic concepts of quantum mechanics; Schrodinger equation; Operators; Commutators; Schrodinger and Heisenberg representations; Particle in a box; Harmonic oscillator; rigid rotor; Solve Schrodinger equation for hydrogen atom; Approximation methods: Variational theorem and perturbation theory; Time-dependent perturbation theory; Spectroscopy; Diatomic molecules; Hartree-Fock; DFT; AI in quantum chemistry.

Course Goals. •Understand the mathematical formalism to describe the behavior of atoms and molecules: quantum chemistry

- Describe the meaning of the wavefunction as it relates to atoms and molecules
- Apply their knowledge on quantum chemistry and wavefunction to solve the Schrodinger equation for simple cases (e.g. harmonic oscillator)
- Explain and apply approximate methods to solve more complex cases (e.g. polyatomic molecules).
- Relate the mathematical knowledge and applications to experimental observables (e.g. spectroscopic signals)

Tentative Schedule of Classes:

| Week | Date | Topic | Homework |
|------|--------|---|------------|
| 1 | Aug 25 | Introduction to the course | |
| 2 | Aug 30 | Dawn of quantum mechanics and classical wave equation | |
| 3 | Sep 6 | Schrodinger Equation and particle in a box | HW 1 |
| 4 | Sep 13 | Postulates of QM, operator, Dirac notation, representations | |
| 5 | Sep 20 | Harmonic Oscillator and rigid rotor | HW 2 |
| 6 | Sep 27 | Angular Momentum | |
| 7 | Oct 4 | Hydrogen atom | Mid term 1 |
| 8 | Oct 11 | Approximation methods | |
| 9 | Oct 18 | Multi-electron system | |
| 10 | Oct 25 | Chemical bonding in diatomic molecules | HW 3 |
| 11 | Nov 1 | Bonding in Polyatomic molecules | |
| 12 | Nov 8 | Computational quantum chemistry | HW 4 |
| 13 | Nov 15 | Group theory and molecule spectroscopy | |
| 14 | Nov 22 | Course Recap | Mid term 2 |
| 15 | Nov 29 | Quantum Chemistry in the era of Artificial Intelligence | |
| 16 | Dec 6 | Project presentation | |

Recommended Textbooks:

Quantum Chemistry by Ira N. Levine

Molecular Quantum Mechanics by P.W. Atkins and R.S. Friedman

Elements of Quantum Mechanics by M. Fayer

Canvas Website. All students will have access to the Canvas website: <https://ufl.instructure.com/>

You will login with your Gatorlink account username and password. This is where you will find general class information, important news, office hours, handouts, class notes, and keys. This is also where you will be able to find out your point totals and histograms.

Class Requirements:

- 1) Four homework (10 points each = 40 points)
- 2) Two midterm examinations (15 points each = 30 points)
- 3) Project presentation (20 points)

4) Attendance and in-class participants (10 points)
= 100 points total

Homework. Homework due date is posted on the class calendar. Late homework (if it is turned in on the same day, but after the 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. You may work in groups or alone. But, you may not copy answers.

Midterm Examinations. There will be two midterm examinations. 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 have to be communicated to the instructor within 48 hrs of the exam and will be considered at the discretion of the instructor.

Project presentation. The frontier research topics related to quantum chemistry will be provided in the middle of the semester, the students can work on the selected projects in teams and present the project at the end of the semester.

Extra Credit. Additional opportunities *should* arise for extra credit (e.g., extensive class participation, attending a lecture outside of class, extra credit quizzes, extra credit problems on the homework, or an extra credit question on an exam). In any event, no more than 50 extra credit points may be earned. Extra credit will be applied after the curve is assigned for the course. This may allow some students to raise their grade by one grade increment (e.g., B+ to A-).

Grading. Grades will be curved based on points earned out of 100. The extra-credit will then be added to those who have earned it to determine if an increase in the final grade is achieved.

Assignment Regrading. If you have a question concerning the grading of an assignment, you may submit the entire assignment for complete regrading. The assignment must be submitted for regrading by the next class meeting after the date the assignment was returned to the class.

Office Hours. Friday morning 10 am, LEI 240C, or by email appointment.

Accommodations for students with disabilities. Students requesting classroom accommodation must first register with the Dean of Students Office. The Dean of Students Office will provide documentation to the student who must then provide this documentation to the Instructor when requesting accommodation.

Course 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 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/>.”

UF Honor Code: 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.”** “The university requires all members of its community to be honest in all endeavors. A fundamental principle is that the whole process of learning and pursuit of knowledge is diminished by cheating, plagiarism and other acts of academic dishonesty. In addition, every dishonest act in the academic environment affects other students adversely, from the skewing of the grading curve to giving unfair advantage for honors or for professional or graduate school admission. Therefore, the university will take severe action against dishonest students. Similarly, measures will be taken against faculty, staff and administrators who practice dishonest or demeaning behavior.”

Cheating and Plagiarism. Cheating and/or plagiarism will not be tolerated. The minimum penalty will be an automatic zero on the assignment in question. Suspension from the University may also result. Do not risk it. It is not worth it. Plagiarism consists of passing off as one’s own the ideas, words, writings, etc. that belong to someone else. You are committing plagiarism if you copy the work of another person and turn it in as your own, even if you have that person’s permission. See: <https://sccr.dso.ufl.edu/policies/student-honor-code-student-conduct-code/>

Copyright Notice. All handouts used in this course are copyrighted and may not be copied without my expressly granted permission. “Handouts” include all materials generated for this class, which include but are not limited to syllabi,

quizzes, exams, problems, in-class materials, lecture note templates, lecture notes, review sheets, problem sets, or other materials. Tutors and tutoring services are expressly forbidden from copying any or all of these materials, unless you pay me two million U.S. dollars. Only students currently enrolled in the class may make a single copy of this material for their personal use.

COVID-19 Statements:

Privacy. Our class sessions may be audio-visually recorded for students in the class to refer 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 verbally 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.

Safety Practices. We will have face-to-face instructional sessions to accomplish the student learning objectives of this course. In response to COVID-19, the following practices are in place to maintain your learning environment, to enhance the safety of our in-classroom interactions, and to further the health and safety of ourselves, our neighbors, and our loved ones.

- If you are not vaccinated, get vaccinated. Vaccines are readily available at no cost and have been demonstrated to be safe and effective against the COVID-19 virus. Visit this link for details on where to get your shot, including options that do not require an appointment: <https://coronavirus.ufhealth.org/vaccinations/vaccine-availability/>. Students who receive the first dose of the vaccine somewhere off-campus and/or outside of Gainesville can still receive their second dose on campus.
- You are expected to wear approved face coverings at all times during class and within buildings even if you are vaccinated. Please continue to follow healthy habits, including best practices like frequent hand washing. Following these practices is our responsibility as Gators.
 - Sanitizing supplies are available in the classroom if you wish to wipe down your desks prior to sitting down and at the end of the class.
 - Hand sanitizing stations will be located in every classroom.
- If you sick, stay home and self-quarantine. Please visit the UF Health Screen, Test & Protect website about next steps, retake the questionnaire and schedule your test for no sooner than 24 hours after your symptoms began. Please call your primary care provider if you are ill and need immediate care or the UF Student Health Care Center at 352-392-1161 (or email covid@shcc.ufl.edu) to be evaluated for testing and to receive further instructions about returning to campus. UF Health Screen, Test & Protect offers guidance when you are sick, have been exposed to someone who has tested positive or have tested positive yourself. Visit the [UF Health Screen, Test & Protect website](#) for more information.
 - Course materials will be provided to you with an excused absence, and you will be given a reasonable amount of time to make up work.
 - If you are withheld from campus by the Department of Health through Screen, Test & Protect you are not permitted to use any on campus facilities. Students attempting to attend campus activities when withheld from campus will be referred to the Dean of Students Office.
- Continue to regularly visit coronavirus.UFHealth.org and coronavirus.ufl.edu for up-to-date information about COVID-19 and vaccination.
- Course materials will be provided to you with an excused absence, and you will be given a reasonable amount of time to make up work. To find more information on the university attendance policies, click here <https://catalog.ufl.edu/UGRD/academic-regulations/attendance-policies/>.