CHEM 542 - Fall 2022
Physical Chemistry: Quantum Mechanics and Spectroscopy

- **Professor**: Sophya Garashchuk
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  In your email message make sure to include "CHEM 542" in your subject line so it can be found in the junkbox.
  Office hours: TBD. I am generally available 9 AM - 4 PM, e-mail to set up an appointment
  TA: Sachith Wickramasinghe sachith@email.sc.edu; GSRC 422; Office hours: TBD

- **Prerequisites**: CHEM 112/142, PHYS 207/212, MATH 241. See your professor if you did not take these courses or did poorly on them. Math skills are crucial for your success in CHEM 542.

- **Text**: Physical Chemistry: Quantum Chemistry and Molecular Interactions, Andrew Cooksy. **Web**: Blackboard CHEM 542

- **Lecture**: Tue Th 1:15-2:30 PM **STB 210** Aug 18 - Dec 2. Important information and changes in the class schedule will be presented in the lecture. Students are responsible for getting notes and information from any missed lectures. An approximate schedule of upcoming material will be given on Blackboard.

  Recitation: Mon 12:00 -12:50 PM **STB 413**. A session for practice of problem-solving techniques through worked examples and occasional quizzes. Student questions and problems are welcome. The problem-solving skills are essential for your success in the course.

  Attendance: mandatory for lectures **and** recitations. Do not leave before the end of a class period unless the instructor has been notified prior to class. See university policy on attendance. Attendance of less than 75% of the lectures will result in F.

- **Homework**: Homework will be assigned approximately once a week and turned in at the beginning of a lecture. Study groups and discussion of the problems with other students, the TA or the instructor are encouraged. However, the material turned in should represent the student's own work and understanding. The homework assignments give a minimum number of problems for the class. Most students will benefit from doing additional problems from the text or other sources (such as sample problems on Blackboard)

- **Midterm Exams**: Sep 22, Oct 20, Nov. 22
  For each exam bring: (i) one-sided 8" x 11" page with your hand-written notes and formulas, (ii) calculator (without preexisting programs), (iii) pencils, (iv) ID card. All other notes, books, programs or other prepared materials may not be used during the test. Calculators may not be shared and must run on batteries. There are no make-up exams. See Final Exam for the policy on missed exams.

  Final Exam: Tue, Dec 08 12:30-3:00 PM

  You may bring four 8"x 11" pages of notes. The exam will be divided into sections corresponding to the material on each of the midterm exams. The score from one and

only one of these sections may be substituted for a missing or low score on one of the midterm exams. This policy will deal with both excused and unexcused absences during the midterm exams.

Last day to drop/withdraw without W is Aug 24

Last day to drop/withdraw without WF is Nov 2

- **Grading**: For both homework and exams, the correct method of solution is more important than the numerical answer. For credit, every answer must be supported by a clear and complete explanation of the method used to find the answer.

  Homework 50 pts + Quizzes 50 pts + Midterms 100 pts each + Final 200 pts = 600

  Following exams, approximate letter grades may be discussed to indicate class ranking. However, final grades will be assigned on the basis of total points.

  The grading scheme (out of 100%):
  $F \leq 50$, $51 \leq D \leq 56$, $57 \leq D \leq 63$, $64 \leq C \leq 70$, $71 \leq C+ \leq 77$, $78 \leq B \leq 84$, $85 \leq B+ \leq 89$, $90 \leq A$.

  All required elements of the course are to be completed within the normal term. Failure to complete all the elements on time will result in a grade of F. Incomplete will only be assigned in unusual circumstances.

- **Graduate Credit**: Additional work outlined in Sec. II must be done to receive graduate credit.

- **Learning outcomes**: Understanding the fundamentals of quantum mechanics. Learning the origin and interpretation of molecular spectra. Understanding of how chemical bonding occurs. Refining the analytical approach to problem solving in general – in class and real world situations.

- **Academic Conduct**: Cheating, plagiarism, copying from old reports, and other forms of academic dishonesty in connection with any portion of this course is a serious infraction and will normally result in failure of the course. Assisting or knowingly cooperating in academic dishonesty will also result in failure in the class. All incidents of academic dishonesty will be reported to the Office of Academic Integrity for possible further disciplinary action.

- **Hazardous Weather**: In case of emergency closure, assignments will be posted on Blackboard. Emergency closures are announced on the university's Carolina alert website `http://carolina alert.edu`

- **Accommodating Disabilities**: Reasonable accommodations are available for students with a documented disability. If you have a disability and may need accommodations to fully participate in this class, contact the Office of Student Disability Services: 777-6142, TDD 777-6744, email `sasds@mailbox.sc.edu`, or stop by LeConte College Room 112A. All accommodations must be approved through the Office of Student Disability Services.

  UofSC attendance policies

  Adhere to the official UofSC guidelines regarding COVID19 mitigation.

Students must attend all classes in the format they are offered (For example, students are expected to attend in-person classes in person). Students who miss classes due to COVID quarantine, a diagnosed health condition or registered disability should contact the Graduate Student Ombudsman (803-777-4243), Prof Wiskur (wiskur(at)mailbox.sc.edu) or Student Disability Resource Services to document the reason for their absence. Students with documented absences may be offered recorded classes, be considered present for participating in class virtually and have the opportunity to reschedule exams, labs or assignments at the instructors discretion; first utilizing any syllabus statement regarding missed class, assignments or exams. EXAMPLE: If the syllabus has a policy on dropping a low or missed exam then that policy will be used for the first missed exam. If a student misses more than one exam with proper official documentation then the second missed exam may be rescheduled. ALL excused absences and accommodations for disabilities MUST have proper official documentation.

I. CLASS SCHEDULE

Updated 08/08/22. I reserve the right to change topics, the order in which they are covered and the midterm exam dates.

1. 8/18: A Introduction: tools from math and physics.
2. 8/23: HW 1. Ch 1 Classical and Quantum Mechanics
3. 8/25: Ch 2 The Schrödinger equation
4. 8/30: HW 2. QM fundamentals
5. 9/1: Uncertainty principle, commutators. Motion in 1D, particle in-a-box
6. 9/6: Particle in 2D- and 3D-box. Separation of variables, degeneracy
7. 9/8: HW 3. Tunneling
8. 9/13 Ch 8 (p. 358) Vibrational motion. Harmonic oscillator, energy levels.
9. 9/15: Vibrational wavefunctions
10. 9/20: HW 4. Ch 3 The one-electron atom. Rotation, the spherical harmonics
11. 9/22: **Midterm I** – Chapters 1, 2, 8 (vibration)
12. 9/27: HW 5. Hydrogenic wavefunctions
13. 9/29: Ionization energy, shells/subshells, selection rules
14. 10/4: HW 6. Electric and Magnetic Dipole Interactions
15. 10/6: Ch 4 Multielectron atom
16. 10/11: HW 7. Spin. Atomic spectra.
17. 10/13-10/14: `Fall break`

18. 10/18: The variation principle and perturbation theory
19. 10/20: **Midterm II** – Chapters 3, 4
20. 10/25: HW 8. Ch 5 Chemical Bonds. Approximate wavefunctions
21. 10/27: Diatomic molecules
22. 11/01: HW 9. Polyatomic molecules
23. 11/03: Computational chemistry
24. 11/08: `Election day`
25. 11/10: HW 10. Ch 8 Vibrational Spectroscopy
26. 11/15: Ch 9 Rotational Spectrosocpy
27. 11/17: HW 11. Ro-vibrational and Raman Spectrosocpy
28. 11/22: **Midterm 3** – Chapters 5, 8, 9
29. 11/29: Ch 6 Molecular Symmetry
30. 12/01: HW 12. Ch 7 Electron spectroscopy. Review.
31. 12/06: TBD Practice session for the final exam
32. 12/08: 12:30-3:00 PM **Final exam** – comprehensive

II. ADDITIONAL ASSIGNMENTS FOR GRADUATE STUDENTS IN CHEM 542

Your grades for these assignments will count as 10% of your overall grade instead of the quiz grades. Discussion problems require at least half a page response. Your work is due one week after we finish with the appropriate chapter.

1. Chapter 1: 1.43, 1.44, 1.45
2. Chapter 2: 2.1, 2.2, 2.29
3. Chapter 3: 3.1, 3.2, 3.3
4. Chapter 7: Anharmonicity of H-H bond. (i) Use Spartan to compute the potential energy curve for H_2 molecule in a singlet state. (ii) Fit the curve to the Morse oscillator form. (iii) Using MAPLE plot the first three eigenstates for the Morse oscillator describing the molecule and the harmonic approximation to this potential. (iv) Compute the overlap of the Morse and for the harmonic oscillator eigenstates with the same quantum number.(v) Extend your MAPLE work (iii-iv) to D_2 molecule. In your writeup, suggest a measure of the anharmonicity of the Morse potential and compare the zero-point energy with and without the anharmonicity for the isotopes considered.

III. COMPUTER LAB RECITATIONS

- Fundamentals of QM – differentiate and integrate with Maple
- Introduction to Spartan – view atomic orbitals, HOMO/LUMO etc
- Vibrational spectroscopy – normal modes of polyatomic molecules and IR spectra using Spartan
- Computational chemistry – build molecules, optimize geometry, compare RHF and DFT dissociation limits for a diatomic molecule