

CHEM 542 - Spring 2016

Physical Chemistry: Quantum Mechanics and Spectroscopy

- **Instructor:** Sophya Garashchuk
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- **Prerequisites:** CHEM 112/142, PHYS 207/212, MATH 241. See instructor 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, 9th Edition, P. W. Atkins (or Part II “Structure” starting with Ch. 7) (8th Edition is acceptable, match the material and homeworks.)
Student Solutions Manual for Physical Chemistry (optional)
Web: Blackboard CHEM 542
- **Lecture:** T Th 11:40-12:66 PM **PSC Jones 006** Jan 12 - Apr 21. 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: W 12:00 PM-12:50 PM **PSC 104**. 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:**
Exam I: Thu, Feb. 18
Exam II: Thu, March. 31
For each exam bring: (i) one-sided 8” x 11” sheet 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: Thu, April 28 at 9:00 AM

You may bring three 8"x11" sheets. 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.

- **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 = 500

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: $A \geq 92$, $B + [86, 92)$, $B[80, 86)$, $C + [74, 86)$, $C[68, 74)$, $D + [62, 68)$, $D[56, 62)$, $F < 56$

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.

I. CLASS SCHEDULE

Updated 01/04/16

1. Jan 12: Introduction, black body radiation, Planck's quantization hypothesis 7.1 (a-b,d). Wave-particle duality, photoelectric effect ($E = h\nu$), electron double-slit experiment, de Broglie wavelength ($\lambda = h/p$)
2. Jan 14: Translational motion, Schrödinger equation, Wavefunctions: (normalization, quantization) 7.4
3. Jan 19: **HW1** Operators, Hermiticity 7.4-5, orthonormal functions
4. Jan 21: Observables, Superposition of eigenstates 7.5-6

5. Jan 26: Uncertainty principle 7.7, commutators, particle in-a-box 8.1
6. Jan 28: **HW2** Particle in-a-box in 2D and 3D, separation of variables, degeneracy 8.2
Tunneling 8.3
7. Feb 2: Vibrational motion, energy levels 9.4, reduced mass (further information 10.1)
8. Feb 4: **HW3** Vibrational wavefunctions, 8.5
9. Feb 9: Rotation in 2D and 3D 8.6, 8.7
10. Feb 11: **HW4** Spin 8.8, Hydrogenic atom, 9.1
11. Feb 16: Energies and wavefunctions 9.2
12. Feb 18: **Midterm I – Chapters 7, 8**
13. Feb 23: Hydrogenic wavefunctions 9.2 (d-g)
14. Feb 25: **HW5** Ionization energy, shells/subshells
15. March 1: Selection rules 9.3. Multielectron atom, The orbital approximation, SCF
9.4-5
16. March 3: **HW6** Linewidth 9.6, singlet and triplet spin states, spin-orbit coupling
9.8-10(a,b)
17. March 7-11: **Spring break**
18. March 15: Variational principle, perturbation theory
19. March 17: **HW7** Valence bond theory 10.1-2
20. March 22: Molecular orbital theory 10.1-4
21. March 24: **HW8** MO for heteronuclear diatomic molecule 10.5, the Hückel approxi-
mation 10.6-7
22. March 29: **HW9** Computational chemistry
23. March 31: **Midterm II, Chapters 9, 10**
24. April 5: Rotational spectroscopy 12.1-5; Boltzmann distribution (further information
15.1-2)
25. April 7 : **HW10** Vibrations of diatomic molecules, selection rules 12.8-9
26. April 12: Anharmonicity, vibration-rotation spectra 12.10-12
27. April 14: Raman spectra 12.10-12
28. April 19: **HW11** Electron spectroscopy, review
29. April 21: Review
30. April 26: TBD Practice session for the final exam
31. April 28: 9:00 AM **Final exam**

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. The first assignment for each chapter calls for a typed (at least half a page) response. Your work is due one week after we finish with the appropriate chapter.

1. Chapter 8

- Discussion question 8.4: compare QM effects for electrons and nuclei.
- Problem 8.15: classical turning point of the harmonic oscillator.
- Problems 8.33 and 8.34: binding of CO to myoglobin.

2. Chapter 9

- Discussion questions 9.8 (the orbital approximation) and 9.9 (effect of the spin-orbit coupling on the spectrum)
- Problem 9.28: Rydberg atoms.

3. Chapter 10

- Discussion questions 10.5 and 10.8: approximations of the Hückel and HF methods.
- Problem 10.27: a study of hydrogen-based 'rings' employing Hückel theory. Also repeat the study using semi-empirical, HF and DFT calculations with at least two different basis sets using Spartan software. Tabulate the energies for all methods/calculations.

4. Chapter 12

- Find and summarize a recent research article pertaining to your research and this course. SCIENCE could be a good source.

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