CHEM 142A: Quantum Mechanics and Spectroscopy  
Spring 2020

Lectures: Tuesdays and Fridays 11:00 AM – 12:20 PM, Volen 106
Instructor: Prof. Rebecca Gieseking  
SSC 3-12  
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781-736-2511
Office hours: Monday 2:30-3:30 PM, Thursday 3:30-4:30 PM, or by appointment
Course website: On LATTE (https://moodle2.brandeis.edu/my/)
Textbook: D. A. McQuarrie and J. D. Simon, “Physical Chemistry: A Molecular Approach.” Reading assignments and any assigned problems will be from the Viva Student Edition. McQuarrie’s “Quantum Chemistry” also includes nearly all the content we will cover, but many section and problem numbers differ.
Ira N. Levine, “Physical Chemistry”, 6th edition, Ch. 17-20  
David J. Griffiths, Introduction to Quantum Mechanics, 2nd edition
Grading: Homework 20% ~10 problem sets
In-class exam 1 25% Tuesday, 2/11
In-class exam 2 25% Tuesday, 3/24
Final exam 30% Date TBD

Course Description and Objectives
The chemical and spectroscopic properties of atoms and the chemical bonds in molecules are primarily due to bound electrons, which behave as described by quantum mechanics, not classical mechanics. In this course, we will describe the basics of quantum mechanics necessary to understand bound electrons and present quantum-chemistry techniques for calculating energy levels and orbitals of atoms and molecules. At the end of this course, you should be able to:

- Explain the differences between classical and quantum mechanics and the limitations of classical mechanics for describing electrons
- Relate the wavefunction to probabilities, averages, and expectation values of observables
- Solve the Schrodinger equation for the wavefunctions of various model systems and be familiar with approximate methods for more complex systems
- Connect the exact wavefunctions of the hydrogen atom to approximate multi-electron solutions for other atoms
- Explain the quantum mechanical origins of covalent bonding and describe the molecular orbitals of diatomic molecules and other simple molecules
- Understand the basic terminology of computational chemistry
• Understand the quantum mechanical foundations of spectroscopy, as related to solutions of the time-dependent Schrodinger equation

Attendance and Reading
Attendance of lectures is expected and is essential for success in this course. Required reading will be assigned before each class.

Homework
Problem sets will typically be assigned on Tuesdays and due in class on the following Tuesday, unless otherwise specified. Late homework assignments will not be accepted unless discussed with the instructor prior to the due date.

I encourage you to discuss homework problems with your fellow students, since this can be a valuable learning tool. However, because the homework is an important tool to gain a thorough understanding of the course material, each student must formulate and write up their answers individually. All work must be legible and presented reasonably neatly and logically.

Exams
There will be two exams during the term and a comprehensive final exam. Exams are closed-book, in the regular classroom, during the regular class period.

Make-up exams will be administered only in exceptional cases due to a documented legitimate conflict (academic, religious, etc.). This conflict must be discussed with the instructor ahead of time or as soon as the conflict is known. In some cases, at the instructor’s discretion, the missed exam may be waived and the final grade will then be based on the other exams and assignments, each taking on a proportionally higher weighting.

Expected Effort
Success in this 4-credit course is based on the expectation that students will spend a minimum of 9 hours of study time per week in preparation for class (readings, homework, studying, etc.).

Cell Phone and Laptop Use
Use of cell phones or laptops in class is prohibited. Note-taking in this course cannot be done effectively using a computer since this course involves many equations and diagrams. If you have extenuating circumstances that require taking notes on a laptop, speak with the instructor.

Students Entitled to Accommodations
Brandeis seeks to welcome and include all students. If you are a student who needs accommodations as outlined in an accommodations letter, please talk with me and present your letter of accommodation as soon as you can. I want to support you.

In order to provide test accommodations, I need the letter more than 48 hours in advance. I want to provide your accommodations, but cannot do so retroactively. If you have questions about documenting a disability or requesting accommodations, please contact Student Accessibility Support (SAS) at 781.736.3470 or access@brandeis.edu.
Academic Integrity

You are expected to be familiar with and to follow the University’s policies on academic integrity. Faculty will refer any suspected instances of alleged dishonesty to the Office of Student Development and Conduct. Instances of academic dishonesty may result in sanctions including but not limited to failure in the course, failure on the assignment in question, suspension from the University and/or educational programs.

Course Topics

Note: order and exact content are tentative.

I. Math and physics background (MathChapters A, B, C, E, F)
II. Foundations of quantum mechanics and 1-dimensional problems
   a. Emergence of quantum mechanics (1.4-1.9)
   b. Schrodinger equation and introduction to particle in a box (3.1-3.8)
   c. Operators, eigenvalues, and expectation values (4.1-4.3, 4.5)
   d. Time evolution (4.4)
   e. Commutation (4.6)
   f. Harmonic oscillator (5.1-5.7)
   g. General principles for 1D wavefunctions
III. Quantum mechanics in three dimensions
    a. Particle in a 3-dimensional box (3.9)
    b. Spherical polar coordinates and rigid rotor (5.8-5.9, MathChapter D)
    c. Hydrogen atom (6.1-6.6)
    d. Many-electron atoms (6.7, 8.1-8.7)
IV. Molecular orbital theory and approximation methods
    a. Variational method (7.1-7.3)
    b. The simplest molecule: H₂⁺ (9.1-9.5)
    c. Molecular orbital theory and chemical bonding (9.6-9.13)
    d. Polyatomic molecules and Hückel theory (10.5-10.6)
    e. Time-independent perturbation theory (7.4)
    f. Computational chemistry methods and terminology
V. Spectroscopy
   a. Time-dependent perturbation theory (13.11)