

CHM 7470: Quantum Chemistry
MWF 11:45–12:40 / 113 State Hall

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Office Hours: MW 1:45–3:00
or by appointment

Course Description and Goals

Quantum mechanics provides a mathematical description of the behavior and interactions of very small particles that are not correctly described by classical mechanics. This course is designed to provide students with the knowledge, theoretical background and mathematical tools to understand theoretical aspects of quantum mechanics and how it is applied to quantum chemistry. Familiarity with undergraduate-level physical chemistry and calculus will be necessary. Students are encouraged to bring issues from their own research (or other interest) to my attention that they would like to discuss. The emphasis should be on the principles of quantum chemistry common to all applications of chemistry. More specifically, at the conclusion of the course you will be able to:

- Define and describe the postulates of quantum mechanics
- Interpret and evaluate literature involving quantum mechanical theory
- Employ analytical or approximate methods to solve the Schrödinger equation for molecular systems and calculate their properties.
- Identify and explain methods employed for quantum chemistry calculations.

However, these goals may be adapted to suit the objectives of the students.

Readings

Required text: *Quantum Chemistry*, 6th Ed., I. N. Levine, Pearson Prentice–Hall Inc., New Jersey, 2009.

This text is on reserve at the science library along with:

Elements of Quantum Mechanics, M.D. Fayer, Oxford University Press.

Molecular Quantum Mechanics, 4th Ed., P. Atkins and R. Friedman, Oxford University Press.

Other recommended texts include :

Mathematics for Quantum Chemistry, J.M. Anderson, Dover.

Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory, A. Szabo and N. S. Ostlund, Dover.

In addition there will be occasional handouts including journal articles. These texts or links to them will be available on the course's Blackboard page.

Course Policies and Evaluation

This course will be interactive in nature; based on this, **attendance** and **participation** will be necessary for you to completely achieve the course goals. Attendance and participation will not be graded directly; however, they are important to the purposes of this course and therefore your active presence in class is expected.

Due to the limited time of the schedule, there will be little time for solving problems in class. However, working through problems and examples is absolutely essential for mastering this subject. You will need to do a significant amount of independent studying in this course, including working through examples and homework problems. I will be available for discussion of the problems during office hours or by appointment.

Evaluation of this course will be based on a variety of in-class and take-home assignments. There will be one mid-term and one final exam. Both exams will be take-home. Besides these exams there will be homework assignments, **posted on Blackboard**. Homework will be due on the date specified in the schedule (below). Another course requirement is a project to be completed individually. This project will be due on the final week of class and will involve a class presentation.

Homeworks, exams and the final project with their respective weights towards the final grade are as follows:

Homework	20% (20 pts.)
Project	20% (20 pts.)
Mid-term exam	25% (25 pts.)
Final exam	35% (35 pts.)

Although some of your evaluation will depend on how well you perform in a test-taking situation, the project will focus on learning as a process of trial-and-error, re-reading and re-thinking. Therefore, parts of the project can be submitted for comments, discussed during office hours and revised prior to the due date. The project will be decided by you and can consist of a presentation of a topic from the current literature related to quantum chemistry or computational chemistry, preferably algorithm/method development.

It is expected that you will abide by the academic integrity requirements as stated in the graduate program requirements document for the department of chemistry. Turn your cell phone, ipod, etc. off during class time. Use of these devices during class is disrespectful to your classmates and myself. Any person using these devices during class will have points deducted off her/his final grade.

If you must miss a class, inform me ahead of time. No late assignments will be accepted and no make-up exams will be given. Deadline extensions may be given for exceptional cases or for religious observance. Excused extensions should be arranged prior to the due date. Learning is a two-way street, therefore, I will ask you for feedback throughout the course. I will take your feedback seriously, and work hard to incorporate your ideas on how to improve the course.

Course Schedule (tentative). Readings key: L=Levine, F=Fayer, AF=Atkins & Friedman

Date	Topics	Readings
9/1	Introduction, historical background	L: 1.1, 1.2; AF: chp. 0
9/3	Superposition and uncertainty principle	L: 1.3; F: chp. 1
9/8	Mathematical interlude	L: 1.6-1.9, 2.1, 5.2
9/10	Operators	L: 3.1-3.2; F: chp. 2 and 4; AF: 1.1-1.2
9/13	Determinants; Problem set 1 due	L: 8.3, 8.4; F 13.A
9/15	Operators, Dirac Notation, Matrix notation	L: 3.3, 7.1-7.4; F: 13.B, chp. 4; AF: 1.3-1.8
9/17	Operators, Dirac Notation, Matrix notation	L: 7.10, 8.6; F: chp. 13.C; AF 1.20-1.24
9/20	Postulates of QM	L: 7.8, 7.9; AF 1.0-1.19
9/22	The Schrödinger eq.	L: 1.4, 1.5; F: 5.A 5.B
9/24	Free particle in 1D	L: 2.3; F: 5.C; AF: 2.1 2.2
9/27	Particle in a box; Problem set 2 due	L: 2.2-2.5; F: 5.D, 5.E; AF: 2.3-2.13
9/29	Harmonic oscillator	L: 4.1, 4.2; F: 6.A, 6.B; AF: 2.16-2.18
10/1	Particle on a ring and rigid rotor	AF: chp. 3
10/4	Molecular vibration; Problem set 3 due	L: 4.3; F: 6.C
10/6	Angular momentum	L: 5.3, 5.4; F: 15.A-15.E; AF: 4.1-4.13
10/8	Angular momentum II	L: 11.1-11.8; F: 15.C-15.E; AF: 4.4-4.13
10/11	Group theory	L: chp 12; AF: chp 5
10/13	Computer lab, class in rm 09 north	
10/15	The Hydrogen atom	L: 6.1-6.4; F: 7.A; AF: 3.9, 3.10
10/18	The Hydrogen atom; Problem set 4 due	L: 6.1-6.4; F: 7.A; AF: 3.11-3.14
10/20	He atom, variational principle	L: 8.1, 8.2; F: 10.B; AF: 6.9-6.10
10/22	Electron spin; Midterm handout	L: 10.1-10.4; F: 16.A, 16.B
10/25	Pauli exclusion principle; Midterm due	L: 10.5; F: 16.C, 16.D, AF: 7.11
10/27	Slater determinants	L: 10.6-10.10
10/29	Molecular structure (Born-Oppenheimer)	L: 13.1-13.5; AF: 8.1-8.2
11/1	Molecular orbital (MO) theory	L: 13.6-13.17; AF: 8.3-8.14
11/3	Hartree-Fock (Roothan-Hall)	L: 11.1-11.2, chp 14; AF: 9.1-9.4
11/5	Hartree-Fock (MO)	L: 15.1-15.9; AF: 9.5-9.6
11/8	Electron correlation; Problem set 5 due	L: 11.3, 16.1; AF: 9.7-9.9
11/10	Moller-Plesset perturbation theory	L: 16.2-13.17; AF: 9.11
11/12	Coupled Cluster Theory	L: 16.2, AF: 9.12
11/15	Density Functional Theory (DFT)	L: 11.3, 16.1-16.3; AF: 9.13-9.14
11/17	Perturbation theory	L: 9.1-9.4 F: 9.A, 9.B; AF: 6.1-6.7
11/19	Perturbation theory	L: 9.5-9.8; F: 9.C; AF: 6.8
11/22	Time-dependent QM; Problem set 6 due	L: 1.4, F: chp 8
11/29	Time-dependent perturbation theory	L: 9.9, 9.10; F: chp 11; AF: 6.11-6.18
12/1	Absorption and emission	F: chp. 12; AF: chps 12 and 13
12/3	presentations	
12/6-12/10	presentations	