CHEM 2430: Quantum Chemistry

Fall 2022

- **Lectures:** *Tue/Thu 5:30-6:45pm, 228* Eberly Hall

- **Office Hours:** *Tuesday and Wednesday 1:00 - 2:00*

The Wednesday office hour will be via zoom. I will give out the zoom link and password in class.

If those times do not work for you, please email me to arrange a meeting time.

- **Professor:** *Kenneth Jordan*

330 Eberly Hall
jordan@pitt.edu

- **Texts:** The main text is:
  - *Quantum Chemistry*

    Ira N. Levine [7th edition (2013)]

***You will also find useful*

  - *Introduction to Quantum Mechanics*

    David J. Griffiths [3rd edition (2018)

COURSE GOALS

Overview:

Chem 2430 is a first-year graduate course in quantum chemistry. The goal of this course is to help students develop a firm conceptual grounding in quantum mechanics and its applications in chemistry.

Key Concepts:

By the end of this course, students will understand and be able to apply

- The properties of operators, the significance of eigenfunctions and eigenvalues and their relationship to experimental observables.
- The role of boundary conditions and their relationship to allowed wave functions.
- How one can transfer the Schrödinger differential eq. to a matrix eigenvalue problem.
- Electron spin, and its consequences for the electronic structure of many electron systems.
- Approximation methods, including the variational method, perturbation theory, the Born-Oppenheimer approximation, Huckel theory, the Hartree-Fock method, and density functional theory.

Systems:

We will explore the key concepts in the context of several fundamental problems of quantum mechanics, including:

- Particles in bound potentials, including square wells, the harmonic oscillators, and the Coulomb potential.
- Particles in unbound potentials and the role of tunneling and resonances.
- Atomic systems, including the hydrogen and helium atoms.
- Simple molecular systems.

Special Topics

I anticipate that we may complete the scheduled topics one or two lectures ahead of schedule. If so, the time freed up will be used to introduce applied quantum chemistry

COURSE STRUCTURE

Grading: There will be three exams, two during the term and each counting toward 27.5 % of the grade, and a final exam worth 35% of the grade. All three exams will be "take home". The remaining 10% of the grade will be based on performance on homeworks.

Problem Sets: Problem sets will be assigned approximately weekly and will be due at the start of class one week after they are assigned.

The homework assignments will enable you to practice and develop your skills as a quantum chemist, and you should dedicate sufficient time to work through the problems. You are allowed to discuss the problem sets with other students in the class; however, each student must write up and turn in their own answers independently.

Exams: Exams will be based on the material from the lectures and the problem sets. All three exams will be take-home to allow you sufficient time to demonstrate mastery of the key concepts. The final exam will be sent to you by the evening of Dec. 9 and should be returned by 5:00 PM on Dec 13. We will not have lectures on Dec. 13 and 15.

Lectures: Course meetings will consist of lectures interspersed with in-class activities, including problems for practice and discussion.

You should read the relevant section of the text in advance of lecture as

I have set up a Piazza web site for the class. Piazza provides an opportunity for you to post questions and to get feedback/clarification on conceptual issues and problem sets. When you post material to Piazza your identity is made known to me but not to other members of the class. I will generally reply to student posts within a few hours.

Classroom Recording: To ensure the open discussion of ideas, students may not record lectures and discussions without the advance permission of the instructor, and any such recording approved in advance can be used solely for the student's own private use. If you have a disability such that you need to record or tape classroom activities, you should contact the Office of Disability Resources and Services (see below) too request an appropriate accommodation.

Academic Integrity: Students in this course will be expected to comply with the University of Pittsburgh's Policy on Academic Integrity (http://www.cfo.pitt.edu/policies/policy/02/02-03-02.html). Any student suspected of violating this obligation for any reason during the semester will be required to participate in the procedural process, initiated at the instructor level, as outlined in the University Guidelines on Academic Integrity.

Disabilities: If you have a disability for which you may be requesting an accommodation, you are encouraged to contact both your instructor and the Office of Disability Resources and Services (http://www.drs.pitt.edu/), 140 William Pitt Union, (412) 648-7890, drsrecep@pitt.edu, (412) 228-5347 for P3 ASL users, as early as possible in the term. DRS will verify your disability and determine reasonable accommodations for this course.

Absences & Make-Up Policy: If you must miss an exam, please contact me as soon as possible so that we can make alternate arrangements. While some exceptions may apply, make-up work (including both problem sets and exams) will generally only be offered in the case of conflicts with religious observances, documented illness and personal or family emergencies.

Use of Canvas: I expect to set up Canvas so that it can be used to submit Homeworks and Exams.

CHEM 2430

FALL 2022

Aug. 30	Chapter I	The Schrodinger Eq.
Sept.. 1, 6	Chapter II	The Particle in a Box
Sept. 8, 13	Chapter III	Operators
Sept. 15, 20	Chapter IV	Harmonic Osc.
Sept. 22	Suppl. Mat.	Harmonic Osc. – with ladder operations
Sept. 27, 29	Chapter V	Angular Momentum
Sept. 29	**Exam 1**	Exam due 10/3 at noon
Oct. 4, 6	Chapter VI	H atom
Oct. 11, 13	Chapter VII	Theorems of QM
Oct. 18, 20	Chapter VIII	Variational Method
Oct. 25, 27	Chapter IX	Perturbation Theory
Nov. 1,3	Chapter X	Electron Spin
Nov. 3	**Exam 2**	Exam due 11/7
Nov 8, Nov. 10	Chapter XI	Many Electron Atoms
Nov. 15 17	Chapter XII	Symmetry
Nov. 29, Dec. 1	Chapter XIV	Theorems Molecular QM
Dec. 6, Dec. 9	Chapter XV	Molecular Electronic Structure
Dec. 9-13	**Take-Home Exam**	