Chemistry 210A
Quantum Chemistry: Introduction & Stationary-State Properties
Winter 2023

Instructor: Prof. Chenchen Song (ccsong@ucdavis.edu)
Lectures: 151 Olson Hall, TR 10:00 – 11:20 AM
Office Hours: Thursday, 2-3PM, Chemistry 190B

TA: Heejune Park (heepark@ucdavis.edu)
TA Office Hours: Tuesday, 2-3PM, Chemistry 190B

Course Webpage: Accessible through Canvas to registered students.
Course Materials: Lecture notes will be uploaded to Canvas after each lecture. In addition, the following books are recommended as references, and are optional.

- Textbook: Helgaker, Jorgensen, Olsen, Molecular electronic structure theory.
- McQuarrie and Simon, Physical Chemistry: A Molecular Approach. Reference for basic quantum mechanics covered in undergraduate level quantum mechanics 110A.
- Szabo and Ostlund, Modern quantum chemistry. Textbook used by previous 210A instructor.

Prerequisites: Preparation in multivariable calculus, differential equations, linear algebra, complex numbers and undergraduate level quantum mechanics (see McQuarrie and Simon in Course materials).

Lecture attendance: Lecture attendance is encouraged. There is no penalty for not attending lecture, but attendance is required during in-class midterm exam (see Exams).

Lecture recordings: Our classroom is "lecture-capture enabled", which allows audio and slides to be recorded, but not boardwork. The recordings will be available on Canvas. According to the instructions I received:

"Links to the recorded lectures will typically appear on your Canvas course site within an hour or two of the end of each class. The videos will appear in "Lecture Videos" and/or "Media Gallery" in the course navigation section of your Canvas course site. We will enable these sections on your site shortly before the start of the quarter."

Topics: This course discusses how time-independent quantum mechanics can be used to study the properties of molecules. Here's a list of topics in roughly chronological order:

1. Postulates of quantum mechanics.
2. Dirac notation and matrix representation of quantum mechanics.
3. Born-Oppenheimer approximation.
4. Harmonic oscillator; normal modes of molecules.
5. Angular momentum; rotations of molecules.
6. Hydrogen atom and spin.
7. Slater determinant; Second quantization and Wick's theorem.
8. Hartree-Fock theory
9. Møller-Plesset perturbation theory
10. Configuration interaction method
11. Multi-reference method

Grading: The point distribution is as: Problem sets 50%, midterm 20%, final 30%.

Problem sets: There will be 5 problem sets. See important dates for post and due dates.

For electronic submissions, please submit to Canvas. Please do not submit through emails as they may get lost.

For physical submissions, please bring to lecture or office hours.

Late problem sets will be accepted until the end of Friday, with a reduced grade of 10% per day late. The reduction in the problem set grade is applied as a percentage taken off points earned. For example, an assignment turned on Thursday (two days late) and graded as 60 points will have 20% of 60 points (i.e. 12 points) taken off for lateness.

Exams: There will be an in-class open-book midterm exam and a take-home final exam (see *Important Dates*). The take-home final is similar to a cumulative problem set but collaboration is not allowed.

Computation and Programming: During the second half of the course, we will be using Psi4 software for performing quantum chemistry calculations through its Python interface.. We plan to give a tutorial about Psi4 during lecture.

Adding/Dropping the Course: Please check the Master Academic Calendar.

Important Dates:

	M	T	W	Th	F
Week 1 (1/9)		Lecture 1		Lecture 2	
Week 2 (1/16)		Lecture 3 PS1 posted		Lecture 4	
Week 3 (1/23)		Lecture 5 PS2 posted PS1 due		Lecture 6	
Week 4 (1/30)		Lecture 7		Lecture 8	
Week 5 (2/6)		Lecture 9 PS3 posted PS2 due		Lecture 10	
Week 6 (2/13)		Lecture 11		Midterm	
Week 7 (2/20)		Lecture 12 PS4 posted PS3 due		Lecture 13	
Week 8 (2/27)		Lecture 14		Lecture 15	
Week 9 (3/6)		Lecture 16 PS5 posted PS4 due		Lecture 17	
Week 10 (3/13)		Lecture 18		Lecture 19	
Final's week (3/20)	Final posted	PS5 due			Final due