Chem-713: Quantum Chemistry: Fall 2022

Instructor: Yuezhi Mao (he/him/his)
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Office location: GMCS 213D (phone #: 619-594-1617)
Lecture Meetings: Tuesday, Thursday 5:00-6:15pm, AH (Adams Humanities)-3150
Practice session: Same as lecture time; location TBA
Office hours: Tuesday 11am-12:30pm, or by appointment
Prerequisite: CHEM-410B, or two semesters of undergraduate P-Chem
Textbook: *Quantum Chemistry*, 7th edition, Ira N. Levine, whose electronic version has been made available through the SDSU Bookstore:
https://shopaztecs.redshelf.com/app/ecom/book/601030/quantum-chemistry-601030-9780133558951-ira-n-levine
(Note: the lecture notes/slides will be more important reading materials since the lectures will not strictly follow the textbook)

General information:

This course is designed to benefit students studying all areas of chemistry and those from other departments who are interested in this discipline. Quantum mechanics governs the motion of microscopic particles including electrons and nuclei, which is underlying almost all chemical phenomena such as bond formation and breaking, molecular interaction, all different types of spectroscopies (UV-Vis, IR, NMR, etc.), and so forth. We will cover two main areas in this course: (i) basic principles of quantum mechanics and its applications to model systems that are relevant to chemistry; (ii) modern electronic structure theory for many-electron systems (primarily molecules). We will have 6 practical sessions, in which students will learn how to write small Python programs to solve model problems and use software to perform quantum chemistry calculations for molecular systems. Students are encouraged to combine what they learn in this course with their own research and to discuss opportunities to employ computational tools in their own research with the instructor.
Note: the instructor will be teaching an Advanced Special Topic Computational Chemistry Course (CHEM-596) in **Spring 2023**, which will focus more on the practical aspects of electronic structure calculations that are left out in this course and cover other topics such as molecular dynamics simulations. We will do some guided reading and discussion of contemporary computational chemistry literature in that course as well. It will be a useful continuation of the CHEM-713 course.

Student learning outcomes:

At the conclusion of this course, the student should be able to:

- Understand the basic concepts and principles of quantum mechanics
- Know how to solve the Schrödinger equation for model systems and apply the solutions (eigenvalues and eigenfunctions) to real chemical systems
- Write down the Schrödinger equation for more complicated chemical systems and tackle the problem using approximate methods

- Program basic linear algebra operations in Python and use Python code to numerically solve quantum mechanical problems
- Understand the idea and practical aspects of electronic structure methods (primarily Hartree-Fock theory and density functional theory)
- Successfully set up electronic structure calculations for molecules using software and accurately interpret the computational results
- Get a sense on the common pitfalls in electronic structure calculations

Tentative course calendar:

Date	**Content**	**Note**
08/23 (Tu)	General introduction; math recap	
08/25 (Th)	More math recap; Schrödinger's equation	Ps1 release
08/30 (Tu)	Particle in box; free particle; particle in rectangular well	
09/01 (Th)	Hilbert space; Dirac's state vector notation; basis expansion	
09/06 (Tu)	Operators; eigenvalues/eigenfunctions; Hermitian operators	Ps1 due
09/08 (Th)	Identify operator; change of basis; x and p operators	Ps2 release
09/13 (Tu)	Practice 1: Introduction to Numpy; basic linear algebra	
09/15 (Th)	Postulates of quantum mechanics	
09/20 (Tu)	Commutating operators; uncertainty principle; superposition and measurements	Ps2 due
09/22 (Th)	1D harmonic oscillators: eigenvalues and eigenfunctions	Ps3 release
09/27 (Tu)	Practice 2: Anharmonicity; Morse potential	
09/29 (Th)	Angular momentum: operators, eigenvalues/eigenvectors	
10/04 (Tu)	Electron spin; Pauli matrices; 2-level system	Ps3 due
10/06 (Th)	The hydrogen atom	Ps4 release
10/11 (Tu)	Variational method: principle and application	
10/13 (Th)	Non-degenerate perturbation theory	
10/18 (Tu)	Degeneracy; Quasi-degenerate perturbation theory	Ps4 due
10/20 (Th)	Practice 3: Variational and perturbative methods in Python	
10/25 (Tu)	Mid-term	
10/27 (Th)	Born-Oppenheimer approximation; Slater determinant	Ps5 release
11/01 (Tu)	Hartree-Fock (HF) theory	
11/03 (Th)	HF in practice; Self-consistent field (SCF) calculations	
11/08 (Tu)	Gaussian basis sets in quantum chemistry	Ps5 due
11/10 (Th)	Practice 4: Hartree-Fock calculations for molecules	Ps6 release
11/15 (Tu)	Introduction to density functional theory (DFT)	Project proposal due/programming template release
11/17 (Th)	Jacob's ladder for DFT functionals	

11/22 (Tu)	Practical consideration for DFT calculations	
11/24 (Th)	No lecture; Happy Thanksgiving!	
11/29 (Tu)	Practice 5: running DFT calculations	Ps6 due
12/01 (Th)	Electron correlation; correlated wavefunction methods	
12/06 (Tu)	Geometry optimization and transition state search	
12/08 (Th)	Practice 6: modeling chemical reactions	
12/13 (Tu)	Final exam (3:30-5:30pm)	
12/16 (F)	Project report due (before mid-night)	

*Ps: problem set

Class project:
Python programming for self-consistent field calculation (with template) or computational study using software (requiring a 1-2 page proposal that is due on Nov. 15); more instructions will be provided.

Grading scheme:
- Homework: 18% (3% each problem set)
- Practice report: 12% (2% each)
- Exams: 50% (mid-term 20%; final: 30%)
- Class project: 20%

Tentative grading scale:
- A: 80-100%
- B: 65-80%
- C: 45-65%

Academic honor code:
Students are expected never to represent someone else's work as their own or assist others in doing so. Violations of this rule will be documented and may result in automatic failure and disciplinary review by the University. Please see the SDSU academic honesty page (https://sacd.sdsu.edu/student-rights/academic-dishonesty/cheating-and-plagiarism) for further information.

Essential student information:
For essential information about student academic success, please see the SDSU Student Academic Success Handbook.
- SDSU provides disability-related accommodations via the Student Ability Success Center (sascinfo@sdsu.edu | sdsu.edu/sasc). Please allow 10-14 business days for this process.
- Class rosters are provided to the instructor with the student's legal name. Please let me know if you would prefer an alternate name and/or gender pronoun.

Land acknowledgment:

For millennia, the Kumeyaay people have been a part of this land. This land has nourished, healed, protected and embraced them for many generations in a relationship of balance and harmony. As members of the San Diego State University community, we acknowledge this legacy. We promote this balance and harmony. We find inspiration from this land, the land of the Kumeyaay.

Diversity, equity, and inclusion:

We, at SDSU, value the diverse identities of our students, faculty, and staff, which include but are not limited to differences in race, gender, ethnicity, sexual orientation, age, socioeconomic status, religion, and disability. We will work together to promote diversity, equity, and inclusion in our learning environment, not only for academic excellence but also for social justice. The instructor is committed to adopt an inclusive teaching approach to help students from different backgrounds succeed in this course. Discussions in which different perspectives are respected and valued are encouraged inside and outside the classroom.