CHEM/QSE 245, Spring 2024
Quantum Chemistry: Theory and Practice

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Course Overview: This course will focus on theoretical and computational quantum chemistry approaches to electronic structure problems in molecules and materials. The mathematical foundation and practical aspects of Hartree-Fock (HF) theory and density functional theory (DFT) will be covered. Advanced methods to treat electron correlation, such as perturbation theory, configuration interaction, and coupled cluster theory, are also discussed. The course will also cover the basics of reaction path study. Finally, if time permits, we will survey other emerging electronic structure methods, including Quantum Monte Carlo, tensor network, and quantum algorithms such as quantum phase estimation. The aim of the course is to prepare students with both fundamental knowledge and practical skills to carry out independent research in the field of quantum chemistry. The project component of the course gives students opportunities to study chemical systems with methods covered in class using Q-Chem software.

Course Objective: After completing the course, students can expect to

- Understand the scaling and the computational feasibility of various quantum chemistry methods for systems of their interest.
- Critically evaluate the computational quantum chemistry calculation data for molecules and extended systems.

Prerequisites: The course is designed for physical chemistry graduate students with knowledge of graduate-level quantum mechanics (e.g., Chem 242). Students from other disciplines (e.g., Physics and QSE) are also welcome. Some background in coding and shell scripting is encouraged but not required.

Lectures: Tuesday 12:00 PM - 01:15 PM, Thursday 12:00 PM - 01:15 PM at Pfizer Lecture Hall in Mallinckrodt Chemistry Lab. Lecture attendance is not mandatory, but highly recommended.

Sections: There will be one section per week on Wednesday 4:30 PM - 5:45 PM (location: TBD) where the TF will cover practical and programming-oriented exercises. In particular, some sections will include hands-on programming components to familiarize students with electronic structure methods and how to run production-level programs for chemical problems. Section is the opportunity to deepen your understanding of the materials covered in the lecture. This time will also cover any missing lectures due to Professor Joonho Lee's travel. TF's office hour will follow the section on Wednesday.

Website: Lecture and section notes, relevant papers, project materials, homework assignments, and solutions (after the due date) will be posted on CHEM 245 canvas.

Problem Set: There will be 8-9 homework assignments throughout the semester. The exact date for each problem set can be found in the schedule. The problem set will include 1-2 problems related to the materials in the last week, 1 Q-Chem and/or 1 coding exercise. All problem sets should be submitted electronically through Gradescope. If you are not familiar with uploading documents to Gradescope, check out this tutorial. The due date for the problem set is 11:59 PM the day specified in the course schedule. Submissions after the deadline will not be accepted.

Exams: The class does not have a final exam. There will be 2 midterms (75 mins) during class time, focusing on the material covered in previous weeks. Students are expected to show up in-person during the exam. All exams are open notes and books, but no internet search is allowed. Exam regrade requests must be submitted no later than a week after the exam score is released.

Project: The material covered in the lectures and sections is designed to help you plan your project. We will go over the detailed description and the expectation for the project in the second half of the course (after spring break). The final project delivery includes a presentation and a written report. The presentation is expected to be during class time and the report due date is at the end of the reading period.

Grading: The grade breakdown is in the table below

	Weight
Problem sets	30%
Exams	50% (25% each)
Project	20%

Class Policies: Students enrolled in the course must read and follow the Honor code. Discussion on homework and term projects with classmates is encouraged. However, students are expected to turn in their own work. Collaboration is strictly prohibited during the exam. Materials used in the final project should be cited properly. Failure to adhere to GSAS policy on academic integrity may lead to a penalty for the corresponding portion of the course.

Generative AI models, such as Bard and ChatGPT, have recently gained popularity in the classroom. We encourage students to experiment with using these AI models to fix code bugs and brainstorm ideas for the final project. ChatGPT can also be a useful tool for writing the final report. However, students should not over-rely on these models for solving homework problems or writing papers since all scientific reasonings/conclusions must stem from accurate and reliable computational calculations.

If students need special accommodations for problem sets, exams, or course projects, they should contact the Disability Access Office (DAO) to request an accommodation letter. Once approved, students should contact class TF to discuss any extensions on course components or accommodation for the exam. Students are encouraged to reach out to Counseling and Mental Health Service if they need mental health support. Other available resources can be found in the Support Resources section on Canvas page.

Textbooks: Here are some helpful textbooks that students are encouraged to read. Most of these textbooks can be reserved from the Harvard Library System. Relevant readings for each week are posted in the course schedule.

- Modern Quantum Chemistry by Szabo and Ostlund (Dover)
- Quantum theory of many-particle systems by Fetter & Walecka (Dover)
- Ideas of Quantum Chemistry Vol. 2 by Piela (3rd edition)
- Introduction to Computational Chemistry by Jensen (3rd edition)
- Density-Functional Theory of Atoms and Molecules by Robert G. Parr and Yang Weitao

Computational resources: Q-Chem jobs used in the course will be carried out using Amazon Web Services (AWS). We will provide more details on how to set up Q-Chem and how to use other software, such as IQmols, to aid with your problem sets and homework when the semester starts.