

Chemistry 883 – Computational Quantum Chemistry

Instructor Contact Information

Professor Benjamin G. Levine

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215 Chemistry Building

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Office Hours

Mondays 9:00-11:00 am in 215 Chemistry or by appointment

Meeting Time and Place

Lecture Sessions – Tues, Thurs 3:00-3:50 pm, 136 Chemistry

Lab Sessions – Wed 1:00-3:50 pm, 336 Chemistry

Online Resources

A course website is available at:

<https://levinegroup.org/teaching/cem-883-computational-quantum-chemistry/>

This site will be used to post the course assignments, lecture notes, and schedule.

Course Content and Objectives

The goal of quantum chemistry (also known as electronic structure theory) is to use computers to approximate the electronic wave function of atoms and molecules and to extract useful information about real chemical systems from that wave function. Such information can include equilibrium structure, thermochemical and kinetic data, and spectroscopic properties. This course is aimed to teach students the basic skills and knowledge necessary to be researchers in quantum chemistry. The specific goals of this course are:

- 1) To introduce students to the hierarchy of methods used to approximate the electronic structure of molecules, the specific applications in which the individual methods are applicable, the circumstances in which they fail, and the reasons underlying their success or failure.
- 2) To introduce students to the language and formalism of quantum chemistry.
- 3) To introduce students to quantum chemical software, specifically Gaussian and Molpro. Students will learn to write an input “deck” (file), run computations on a typical computer cluster, and interpret the resulting output.
- 4) To encourage students to critically analyze and communicate their results like researchers in computational chemistry.

Course material will be presented through a combination of readings, lectures, and hands-on exercises (labs). In general, readings will be used to present formalism; lectures will be used to underline concepts and develop intuition from the formalism; and labs will be used to teach practical skills and reinforce important concepts. A basic understanding of undergraduate-level quantum mechanics is assumed.

Course Topics and Approximate Schedule

Lectures will cover the following topics:

- An Intro to Quantum Chemistry and Potential Energy Surfaces
- Superposition, The Matrix Representation of Quantum Mechanics, and Basis Sets
- The Hartree-Fock Approximation
- Introduction to Wave Function-based Approaches to Electron Correlation
 - Configuration Interaction
 - Moller Plesset Perturbation Theory
 - Coupled Cluster
- Basis Set Superposition Error
- Density Functional Theory
- Semiempirical Methods
- Multireference Methods (if time allows)
- Excited States (if time allows)
- Ab Initio Molecular Dynamics (if time allows)
- Introduction to High Performance Computing (if time allows)

Lab exercises will cover the following topics:

- The Basics of Running Gaussian and Molden
- Simple Calculations on Small Molecules
- Theoretical IR and NMR Spectroscopy
- Dynamic Electron Correlation
- Potential Energy Surfaces
- Theoretical UV-VIS Spectroscopy

Grading Policy

The semester grades will break down as follows:

60% Homework

30% Final Project

10% Final Exam

Homework assignments will be made after each lab exercise is complete. They will include both mathematical and qualitative questions. In either case, your explanation is expected to be clearly

written in complete sentences and/or equations. Write as if you are trying to communicate the material to someone who does not already know it. You may need to include figures or tables containing data produced in the lab exercise.

Your final project will include two stages. In the first stage, you will choose a scientific paper from a reputable journal (for example, the Journal of Physical Chemistry, Journal of Chemical Physics, Journal of Chemical Theory and Computation, or the Journal of the American Chemical Society) that contains electronic structure calculations. You will write a roughly one-page review of this paper, summarizing the key results, providing critical feedback on the study, and suggesting some calculations that could extend the study. In the second stage you will perform that calculations that you proposed and write a lab report describing the results. Due dates will be set during the semester for these two projects.

The final exam is scheduled for Wednesday December 12 10:00-12:00 in Chemistry 136. The final exam will cover the material presented on the homework and in the lab exercises.

Lab Report

To write a good lab report one should:

1) Write in the style of a short scientific article, such as one would see in a reputable scientific journal. The report should be organized into sections:

- a) A very brief Introduction section should describe the problem being approached.
- b) The methods used should be described in the Methods section. The goal is to describe what you have done such that another reasonably knowledgeable scientist could reproduce it. This means telling what software you used, what methods, and what the parameters of those methods were. You are not required to include equations describing the methods unless specifically noted.
- c) A Results and Discussion section describes the results of the calculations you did, why those results are what they are, and what those results mean. It should present them in a fashion that is easily understood by the reader. Generally this means condensing the information into a small number of figures and/or tables. Do not simply reword the Gaussian output file, but discuss why the results are the way they are. Note that results and discussion are two different things, even if they are lumped together into one sections. Results answer the question “what is the result of the calculation?” Discussion answers the questions “why was the result the way that it was?” or “what is the meaning of this result in the broader context of the field?” Both results and discussion should be included. When writing discussion ask yourself “why did Ben ask me to do this calculation? What was I supposed to learn here? How does this relate to what we’ve learned in lecture?”
- d) A very brief Conclusion section should summarize the key results of the exercise.

2) Be brief. A longer report is not a better report. Only include information relevant to the conclusions you are drawing.

3) Be clear. Your goal is to communicate to someone who already knows something about quantum chemistry what you did and what you observed as a result.

4) Revise and proofread. Spelling and grammatical errors, unclear language, and poorly organized thoughts undermine your attempt to communicate your results. I strongly encourage you to make use of the MSU Writing Center (<http://writing.msu.edu>) and English Language Center (<http://elc.msu.edu>) to improve your writing.

5) Figures and tables should be formatted neatly. All axes and quantities should be labeled. Use units familiar to both theorists and experimentalists (e.g. Angstrom, eV, kcal/mol, or cm^{-1}) unless there is a good reason to use atomic units (e.g. Bohr, Hartree). Clearly label all units. Make sure to interpret all figures in the text.

Lab reports **SHOULD NOT** include the Gaussian or Molpro output in its entirety or in part. The output is an intermediate in the process of doing science, but it is not how you communicate science to others. One of the most important parts of your job is to interpret the raw data and put it into context.

Late Work

Assignments are due in class on the stated due date, which will be mentioned at the beginning of class. Assignments can be submitted in hard copy or by email. I will respond to acknowledge assignments submitted by email. If you don't get a response, it means that I did not get it, and it is your responsibility to make sure that I do. Late assignments can be turned in up to two weeks late or before the final exam, whichever is earlier. The first time you are late (by less two weeks) you will get full credit, but subsequent late assignments will receive one half credit. No assignment more than two weeks late will receive credit.

Collaboration and Plagiarism

Your classmates, labmates, etc. are excellent resources to learn from. I encourage you to discuss both technical issues (running the calculations) and scientific ones (interpreting the results) with each other. However, every student in the class is responsible for running their own calculations and writing their own lab report.

If you use the work of another in writing your paper (for example, but not limited to, a published paper or book), it should be cited properly. Failure to do so is plagiarism, which is not tolerated in the scientific community and will not be tolerated in this class. Plagiarism may result in failure of the course. If you are in doubt about whether your actions constitute plagiarism, please ask. Additional information about academic dishonesty at MSU can be found at <https://www.msu.edu/unit/ombud/dishonestyFAQ.html>

Attendance

Attendance at all lecture and laboratory periods is expected. Let me know in advance if you will be missing class for a good reason. Excessive and/or unexcused absence may result in reduction of your final grade.

Readings

Required text: Modern Quantum Chemistry, by Szabo and Ostlund – This is the most widely used text on the formalism of traditional, wave function-based electronic structure theory, and it's inexpensive too (~\$15 on Amazon.com). Every single quantum chemist owns and has read this one. It is a little dated and can be challenging for beginners, but the earlier you read it the better.

When material is not covered by Szabo and Ostlund, I will pass out required readings drawn from a variety of sources. Many of these readings will be taken from the following books, which are not required, but recommended:

Essentials of Computational Chemistry, by Cramer – This is a less rigorous, but more readable text on computational chemistry in general. This book is good for giving you the basic idea behind a topic before using Szabo and Ostlund to fill in the details.

Methods of Molecular Quantum Mechanics, by McWeeny – Similar to Szabo and Ostlund, but gives a superior treatment of valence bond and multireference methods. (It is out of print, so it can be difficult to find.)

A Chemists Guide to Density Functional Theory, by Koch – A thorough but accessible introduction to DFT. My presentation of DFT in this class is based on Koch's presentation in this book.

Elements of Quantum Mechanics, by Fayer – This is a textbook on graduate level quantum mechanics which is noteworthy for its conciseness (it's barely 300 pages long) and clarity.