Instructor  
Sara E. Mason, Ph.D. (SEM)  
Office: W339 CB  
Phone: (319) 335-2761  
Email: sara-mason@uiowa.edu

SEM Office Hours  
In W339 CB, Wednesday 2-4 PM, Thursday 3:30-4:30 PM  
or by appointment.

Department DEO  
Prof. James Gloer  
Administrative Office: E331 CB  
Administrative Phone: (319) 335-1350  
Administrative Email: chem-dept@uiowa.edu

Lecture  
2-3:15 PM TTH, in room 215 PH.

Text  
No specific text is assigned. Course readings will be provided through ICON and/or materials put on reserve.

Website  
http://icon.uiowa.edu

Course Objectives  
Fundamental principles of quantum chemistry; angular momentum; approximation methods; theory of atomic and molecular electronic structure; applications of computational quantum mechanics to chemical systems.

Grading  
Exam 1  
Exam 2  
Problem Sets  
Project  

25%  
25%  
30%  
20%

If you have questions about your grade status, please see an instructor during office hours or by appointment.

Final grades will use + and - designations, with A+ reserved for truly exceptional cases.
**CHEM:5433 Quantum and Computational Chemistry, Spring 2017**

**Prerequisites and Required Background Material**
The listed co-requisite for this course is CHEM:4432, which is the semester of undergraduate chemistry that introduces quantum mechanics. It is the case that this class is made up of a variety of backgrounds. As such, I will make every effort to (re)introduce important mathematical and physical concepts before they are used in class. It is also the case that you will need to use various mathematical and/or quantum mechanical software in this class. I will attempt to offer tutorials and background on how to use the software, but it will be up to you to make sure you ask for help if you are stuck.

**Attendance**
Attendance is optional. All lectures will be posted online, in video and/or note form, shortly after class. Further details about how to access course videos will be provided on ICON.

**Cell Phones and Personal Electronic Devices**
I request that you abstain from unnecessary use of cell phones and other personal electronic devices during class.

**Exams**
Exams will not be given during class time. Instead, both exams will be given in take-home format. More details on the exam format will be given within two weeks of the first exam.

**Timely Completion of Assignments**
Problem sets that are not turned in on time are subject to a grade penalization as seen fit by the instructor.

**Expectations for the Completion of Problem Sets**
The problem sets are an integral part of this course. You can discuss the problem sets with your peers. However, copying work is not discussion. All written work must be individually prepared. Work that is copied from another student is not acceptable. Please see the section in the Student Academic Handbook on Rights and Responsibilities for University policy on academic misconduct. You are encouraged to seek out references to assist in solving the problems, as necessary. If you use a source in your solution, make sure you detail your work enough so that I believe that you thoroughly understand all of the steps. Also clearly cite any references you use.
CHEM:5433 Quantum and Computational Chemistry, Spring 2017

When answering a question, one needs to know he audience for the answer. In preparing problem set solutions, direct your answers towards a classmate who is “somewhat behind” you in terms of studying. Your solutions to each problem set should be detailed enough to serve as a study aid to another student in class whose understanding of the materials is less proficient than your own. Err on the side of explaining a little too much, or showing a bit too much work. Also be sure that your solutions are easily readable and that you use the same symbols/notation as used in class and in the text. This will ensure that you receive optimal point credit for your solutions. You will be given feedback, if necessary, on the quality of your problem set solutions. If you fail to address that feedback in subsequent assignments, you will lose points accordingly.

ProjectDetails of the course project will be provided later in the semester. Briefly, the projects will be done independently and outside of class. Each student will select a project, either based on my suggestions or the student’s own ideas, subject to my approval. Projects can be either programming-based (so long as the program is developed to explore a quantum mechanical problem) or computational (such as using a software that performs quantum chemical methods).

Safe Zone Statement
I am part of the Safe Zone Project community network of trained University of Iowa faculty/staff/students who are available to listen and support you in a safe and confidential manner. My goal is to help you be successful and to maintain a safe and equitable campus. The purpose of the Safe Zone Project is to identify members of the University community who will model support, affirmation, and inclusion of LGBTQ people. Participants who complete this program are choosing to be visible allies and to be trained to be effective resource people for their workplace and classroom.

I want to emphasize again that if you have any questions or concerns, please communicate those to me so that I can help you. I am available and I will be happy to talk with you.
CHEM:5433 Quantum and Computational Chemistry, Spring 2017

Administrative Home
The College of Liberal Arts and Sciences is the administrative home of this course and governs matters such as the add/drop deadlines, the second-grade-only option, and other related issues. Different colleges may have different policies. Questions may be addressed to 120 Schaeffer Hall, or see the CLAS Academic Policies Handbook at http://clas.uiowa.edu/students/handbook.

Electronic Communication
University policy specifies that students are responsible for all official correspondences sent to their University of Iowa e-mail address (@uiowa.edu). Faculty and students should use this account for correspondences. (Operations Manual, III.15.2. Scroll down to k.11.)

Accommodations for Disabilities
A student seeking academic accommodations should first register with Student Disability Services and then meet with the course instructor privately in the instructor’s office to make particular arrangements. See http://sds.studentlife.uiowa.edu/ for more information.

Academic Honesty
All CLAS students or students taking classes offered by CLAS have, in essence, agreed to the College’s Code of Academic Honesty: "I pledge to do my own academic work and to excel to the best of my abilities, upholding the IOWA Challenge. I promise not to lie about my academic work, to cheat, or to steal the words or ideas of others; nor will I help fellow students to violate the Code of Academic Honesty.” Any student committing academic misconduct is reported to the College and placed on disciplinary probation or may be suspended or expelled (CLAS Academic Policies Handbook).

CLAS Final Examination Policies The final examination schedule for each class is announced by the Registrar generally by the fifth week of classes. Final exams are offered only during the official final examination period. No exams of any kind are allowed during the last week of classes. All students should plan on being at the UI through the final examination period. Once the Registrar has announced the date, time, and location of each final exam, the complete schedule will be published on the Registrar’s web site and will be shared with instructors and students. It is the student’s responsibility to know the date, time, and place of a final exam.

Making a Suggestion or a Complaint Students with a suggestion or complaint should first visit with the instructor (and the course supervisor), and then with the departmental DEO. Complaints must be made within six months of the incident (CLAS Academic Policies Handbook).
Understanding Sexual Harassment
Sexual harassment subverts the mission of the University and threatens the well-being of students, faculty, and staff. All members of the UI community have a responsibility to uphold this mission and to contribute to a safe environment that enhances learning. Incidents of sexual harassment should be reported immediately. See the UI Office of the Sexual Misconduct Response Coordinator for assistance, definitions, and the full University policy.

Reacting Safely to Severe Weather
In severe weather, class members should seek appropriate shelter immediately, leaving the classroom if necessary. The class will continue if possible when the event is over. For more information on Hawk Alert and the siren warning system, visit the Department of Public Safety website.

*These CLAS policy and procedural statements have been summarized from the web pages http://www.clas.uiowa.edu/ of the College of Liberal Arts and Sciences and The University of Iowa Operations Manual.