CHEM:4480:001 Introduction to Molecular Modeling
Fall 2018

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

Lecture
11:00 AM - 12:15 PM, Tuesday/Thursday. Primary Location: W228 CB. Please note that we will often meet in one of the Chemistry Computer Labs. Notice about class being held outside of the primary location will be posted to the course ICON site by 24 hours prior to the start of class.

Office Hour
Tuesday 12:30-2 PM (EXCEPT for DoC faculty meeting days 9/4, 10/2, 10/9, 11/6, and 12/4), Thursday 12:30-2, or by appointment

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

Text
Instead of a course text, assigned readings will be given throughout the semester in forms such as journal articles or library reserves.

Website
http://icon.uiowa.edu

Course Objectives
To develop practical skills associated with chemical modeling based on quantum mechanics and computational chemistry such as working with shell commands, mathematical software, and modeling packages. We will also work to develop a basic understanding of quantum mechanics, approximate methods, and electronic structure. Technical computing, pseudopotential generation, density functional theory software, (along with other optional packages) will be used hands-on to gain experience in data manipulation and modeling. We will use both a traditional classroom setting and hands-on learning in computer labs to achieve course goals.

Course Topics
• Introduction: It’s a quantum world!
• Dirac notation and matrix mechanics (a.k.a. Bras, kets, and all of that)
• Solving the Schrödinger equation
• Hands On: Aufbau principle and periodic trends through atomic all-electron calculations
• Potential Energy Surfaces
• Hands On: Setting up molecules for quantum chemical calculations in Spartan
• Hartree Fock Theory
• Science Communication
• Hands On: Geometry optimizations and physical properties in Spartan
• Variational principle and perturbation theory
• Hands On: Numerical solution of the harmonic oscillator in Maple
• Density Functional Theory and Materials Design
• Hands On: Quantum Espresso tutorials
• Special Topics in Quantum Chemistry in Nano, Environmental, and Energy Chemical Sciences
• Hands On: Class/team project: In silico study of doped semiconductors

Grading

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<thead>
<tr>
<th>Component</th>
<th>Percentage</th>
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<tbody>
<tr>
<td>Homework</td>
<td>35%</td>
</tr>
<tr>
<td>In-class work and participation</td>
<td>30%</td>
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<tr>
<td>Quizzes</td>
<td>10%</td>
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<tr>
<td>Contribution to class/team project</td>
<td>25%</td>
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<tr>
<td>Final course grades will use ± designation.</td>
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Prerequisites and Required Background Material
The co-requisite for this course is CHEM:4432 (Physical Chemistry II). Throughout the course, I will make an effort to review the key mathematical and quantum mechanical concepts required to appreciate the course material, but the basics of quantum mechanics is required as background material.

Expected Student Workload
This is a 3 credit hour course, so under University policy you should expect to spend six hours per week outside of class on activities related to this course.

Attendance
Attendance is expected, and as noted above, in-class work and participation contribute to your grade. Communicate necessary absences to me as soon as possible so that we can agree on how you will make up any missed work. Please use common sense and courtesy regarding cell phone/personal electronics Use in class.

Expectations for the Completion of Assignments
You may discuss and work on all assigned work in groups if you wish. You may also consult any references (textbooks, online, journal articles...) to aid in completing assigned problems. However, I require each student to hand in a separate and unique solutions. When preparing your individual solutions, prepare them as if they are to be used by another student in class as a study guide. That is, regardless of your understanding of the material, write your solutions for a student who is a “bit behind” you in their understanding. In other words, do not think of *me* as your audience, consider your audience to be a classmate you are trying to teach. If you consult an outside source, please provide a reference and explain how that source aided in your solution and/or understanding. Some class time is used for hands-on computational work or problem solving, and we will often work in, and/or hold discussions in, small teams.
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 that if you have any questions or concerns, please communicate those to me so that we can work towards a resolution. I am available and welcome you to talk with me.

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).

Accommodations for Disabilities
UI is committed to an educational experience that is accessible to all students. A student may request academic accommodations for a disability (such as mental health, attention, learning, vision, and physical or health-related condition) by registering with Student Disability Services (SDS). The student should then discuss accommodations with the course instructor http://sds.studentlife.uiowa.edu/.

Nondiscrimination in the Classroom
UI is committed to making the classroom a respectful and inclusive space for all people irrespective of their gender, sexual, racial, religious or other identities. Toward this goal, students are invited to optionally share their preferred names and pronouns with their instructors and classmates. The University of Iowa prohibits discrimination and harassment against individuals on the basis of race, class, gender, sexual orientation, national origin, and other identity categories set forth in the University’s Human Rights policy. For more information, contact the Office of Equal Opportunity and Diversity at diversity@uiowa.edu or diversity@uiowa.edu.

Academic Integrity
All undergraduates enrolled in courses offered by CLAS have, in essence, agreed to the College’s Code of Academic Honesty. Misconduct is reported to the College,
resulting in suspension or other sanctions, with sanctions communicated with the student through the UI email address.

**CLAS Final Examination Policies**
The final exam schedule for each semester is announced around the fifth week of classes; students are responsible for knowing the date, time, and place of a final exam. Students should not make travel plans until knowing this final exam information. No exams of any kind are allowed the week before finals. ([https://clas.uiowa.edu/faculty/teaching-policies-resources-examination-policies](https://clas.uiowa.edu/faculty/teaching-policies-resources-examination-policies))

**Making Complaint**
Students with a complaint should first visit with the instructor or course supervisor and then with the departmental executive officer (DEO), also known as the Chair. Students may then bring the concern to CLAS ([https://clas.uiowa.edu/students/handbook/student-rights-responsibilities](https://clas.uiowa.edu/students/handbook/student-rights-responsibilities)).

**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 must uphold the UI mission and contribute to a safe environment that enhances learning. Incidents of sexual harassment must be reported immediately. For assistance, definitions, and the full University policy, see [https://osmrc.uiowa.edu/](https://osmrc.uiowa.edu/).