CHEM:4480:001 Introduction to Molecular Modeling
Fall 2021

Instructor
Dr. Sara E. Mason
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Lecture
11:00 AM - 12:15 PM, Tuesday/Thursday. Location: 118 MH. Please note that we will often meet in one of the Chemistry Computer Labs, W238 CB. Notice about our meeting location will be posted to the course ICON site at least 12 hours prior to the start of class.

Office Hours
Monday 10:30-11:30 AM, Thursday 12:15-1:15 PM, Friday 10:00-11:00 AM, or by appointment.

Department DEO
Dr. Leonard R. MacGillivray
Administrative Office: E331 CB
Administrative Phone: (319) 335-1350
Administrative Email: chem-admin@uiowa.edu

Text
Instead of a course text, assigned readings will be given throughout the semester in forms such as journal articles or scanned 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. Symbolic and numeric computing, programming, and density functional theory software 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
- Potential Energy Surfaces
- Hartree Fock Theory
- Science Communication
- Variational principle and perturbation theory
- Density Functional Theory and Data-Driven Materials Design
• Special Topics in Quantum Chemistry in Nano, Environmental, and Energy Chemical Sciences
• Hands On: Linear algebra and symbolic math in Maple
• Hands On: Numerical methods and programming in Maple
• Hands On: Aufbau principle and periodic trends through atomic all-electron calculations
• Hands On: Quantum Espresso tutorials
• Hands On: Class/team project: Nanomaterial transformations in the environment: Mechanistic studies of cation release from complex metal oxides and data-driven model development

Grading

<table>
<thead>
<tr>
<th>Component</th>
<th>Percentage</th>
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<tbody>
<tr>
<td>Homework</td>
<td>35%</td>
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<tr>
<td>In-class work and participation</td>
<td>30%</td>
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<tr>
<td>Quizzes</td>
<td>10%</td>
</tr>
<tr>
<td>Contribution to class/team project</td>
<td>25%</td>
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</tbody>
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Final course grades will use ± designation.

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 and you should expect to spend six hours per week outside of class on activities related to this course. If you are experiencing a higher demand than this, please feel free to bring this to my attention during office hours (or by appointment). I am happy for feedback and to offer suggestions to manage the coursework.

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._
ATTENDANCE AND CLASSROOM EXPECTATIONS
Students are responsible for attending class and for knowing an instructor’s attendance policies, which vary by course and content area. All students are expected to attend class and to contribute to its learning environment in part by complying with University policies and directives regarding appropriate classroom behavior or other matters.

ABSENCES
Students are responsible for communicating with instructors as soon they know that an absence might occur or as soon as possible in the case of an illness. Delays in communication could result in a forfeit of what otherwise might be an excused absence.

ABSENCES: ILLNESS, UNAVOIDABLE CIRCUMSTANCES, AND UNIVERSITY SPONSORED ACTIVITIES
Students who are ill, in an unavoidable circumstance affecting academic work, or who miss class because of a University sponsored activity are allowed by UI policy to make up a missed exam. Documentation is required by the instructor except in the case of a brief illness. Students are responsible for communicating with instructors as soon as the absence is known (https://opsmanual.uiowa.edu/students/absences-class#8.1).

ABSENCES: HOLY DAYS
Reasonable accommodations are allowed for students whose religious holy days coincide with their classroom assignments, tests, and attendance if the student notifies the instructor in writing of any such religious Holy Day conflicts within the first days of the semester and no later than the third week. (See the University Operations Manual: https://opsmanual.uiowa.edu/students/absences-class#8.2).

ABSENCES: MILITARY SERVICE OBLIGATIONS
Students absent from class due to U.S. veteran or U.S. military service obligations (including military service-related medical appointments, military orders, and National Guard Service obligations) must be excused without penalty. Instructors must make reasonable accommodations to allow students to make-up exams or other work. Students must communicate with their instructors about the expected possibility of missing class as soon as possible. (For more information, see https://opsmanual.uiowa.edu/iv-8-absences-class%C2%A0-0).

ACADEMIC MISCONDUCT
Plagiarism and the process for addressing academic misconduct of graduate students are defined in Section IV, Article F “Plagiarism by Graduate Students” of the UI Graduate College Manual of Rules and Regulations. Please contact the CLAS Associate Dean for Graduate Education for any necessary assistance in navigating the process mandated by the Graduate College.

ACADEMIC ACCOMMODATIONS
UI is committed to providing an educational experience that is accessible to all students. A student may request academic accommodations for a disability (such as a mental health, attention, learning, vision, and a physical or health-related condition) through the Student Disability Services (SDS) office. The student is responsible for discussing specific accommodations with the instructor. Note that accommodations are not granted retroactively but from the time of the student’s request to the instructor onward; additionally, accommodations must be requested at least two weeks in advance of the related assignment or exam (https://sds.studentlife.uiowa.edu/). Graduate students serving as Teaching Assistants, Research Assistants, or Fellows must contact Faculty and Staff Disability Services (https://hr.uiowa.edu/support/faculty-and-staff-disability-services) for assistance with accommodations.

CLASS RECORDINGS: PRIVACY AND SHARING
Course lectures and discussions are sometimes recorded or live-streamed. These are only available to students registered for the course and the intellectual property of the faculty member. These materials may not be shared or reproduced without the explicit written consent of the instructors. Students may not share these recordings with those who are not enrolled in the course; likewise, students may not upload recordings to any other online environment. Doing so is a breach of the Code of Student Conduct and could be a violation of the Federal Education Rights and Privacy Act (FERPA); also see https://dos.uiowa.edu/policies/code-of-student-life/.
COMMUNICATION: UI EMAIL
Students are responsible for all official correspondences sent to their UI email address (uiowa.edu) and must use this address for any communication with instructors or staff in the UI community (Operations Manual, III.15.2). Emails should be respectful and brief, with complex matters addressed during the instructor’s drop-in hours, for example. Faculty are not expected to answer email after business hours or during the weekends.

FREE SPEECH AND EXPRESSION
The University of Iowa supports and upholds the First Amendment protection of freedom of speech and the principles of academic and artistic freedom. We are committed to open inquiry, vigorous debate, and creative expression inside and outside of the classroom. Visit Free Speech at Iowa for more information on the University’s policies on free speech and academic freedom: https://freespeech.uiowa.edu/.

COMPLAINTS ABOUT ACADEMIC MATTERS
Students with a complaint about a grade or a related academic matter should first visit with the instructor and then with the course supervisor (if applicable), and finally with the director of the school, department, or program offering the course. If a graduate student has not been able to resolve the issue through the director of the school, department, or program, they should contact the associate dean for graduate education in the College of Liberal Arts and Sciences.

FINAL EXAMINATION POLICIES
The final exam schedule is published during the fifth week of the fall and spring semesters or on the first day of summer classes; students are responsible for knowing the date, time, and place of their final exams. Students should not make travel plans until knowing this information. A student with exams scheduled on the same day and time or who have more than two final exams on the same day should visit this page for how to resolve these problems by the given deadline (https://registrar.uiowa.edu/makeup-final-examination-policies). No exams are allowed the week before finals, but with some exceptions made for labs, language courses, and off-cycle courses (https://registrar.uiowa.edu/final-examination-scheduling-policies).

HOME OF THE COURSE
The College of Liberal Arts and Sciences (CLAS) is the home of this course, and CLAS governs the policies and procedures for its courses. Graduate students, however, must adhere to the academic deadlines set by the Graduate College. See https://grad.uiowa.edu/academics/deadlines.

MENTAL HEALTH
Students are encouraged to seek help as a preventive measure or if feeling stressed or overwhelmed. Students should talk to their instructors for guidance with specific class-related concerns and are encouraged to contact University Counseling Service (UCS) at 319-335-7294 during regular business hours to schedule an appointment. UCS offers group and individual therapy as well as counseling for couples about relationships while making referrals to other resources (https://counseling.uiowa.edu/). Student Health can also address related concerns (https://studenthealth.uiowa.edu/). These visits are free to students. After hours, students are encouraged to call the Johnson County Community Crisis Line at (319) 351-0140 or dial 911 in an emergency.

NONDISCRIMINATION IN THE CLASSROOM
The University of Iowa is committed to making the classroom a respectful and inclusive space for people of all gender, sexual, racial, religious, and other identities. Toward this goal, students are invited in MyUI to optionally share the names and pronouns they would like their instructors and advisors to use to address them. The University of Iowa prohibits discrimination and harassment against individuals based on race, class, gender, sexual orientation, national origin, and other identity categories indicated by the University’s Human Rights policy. For more information, contact the Office of Equal Opportunity and Diversity at https://diversity.uiowa.edu/division/office-equal-opportunity-and-diversity-eod.

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 are expected to conduct themselves in a manner that maintains an environment free from sexual harassment and sexual misconduct. Those experiencing Incidents of sexual harassment are strongly encouraged to report incidents and to seek help (https://osmrc.uiowa.edu/).