CHEM:4480:001 Introduction to Molecular Modeling
Fall 2015

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: C139 PC. 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
TBA, or by appointment

Department
Dr. Daniel M. Quinn
DEO
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 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 Content
• Introduction: What is computational chemistry and where do we start?
• Learn by doing linear algebra in Maple
• Dirac notation and matrix mechanics
• Solving problems numerically
• Structure of the nonrelativistic molecular Hamiltonian
• Setting up molecules for quantum chemical calculations in Spartan
• Geometry optimizations and physical properties in Spartan
• Variational principle and perturbation theory
• Solving exact and perturbed quantum harmonic oscillators in Maple
- Hartree-Fock theory and quantum chemical methods
- Shells for command line computing and scripting
- Atomic pseudopotentials using OPIUM
- Density functional theory (DFT)
- Quantum Chemistry in Nano, Environmental, and Energy Chemical Sciences

### Grading

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<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>25%</td>
</tr>
<tr>
<td>Quizzes</td>
<td>15%</td>
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<tr>
<td>Final project/oral presentation</td>
<td>25%</td>
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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, 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. Use of cell phones during class will forfeit your attendance for that class, and thus you will receive a zero on any quiz or in-class assignment for that day. If you are in a situation that requires that you check your phone during class (such as, if you are on high alert for a family emergency), then please email or meet with me privately so that I can exempt you from this policy as necessary.

### Expectations for the Completion of Assignments

You may discuss problem sets as a group and you may consult any references 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. If you consult an outside source, please provide a reference and explain how that source aided in your solution and/or understanding. When class time is used for hands-on computational work or problem solving, you may work in groups but every person is responsible for submitting their own work individually.

*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, 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 Fraud
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.