CHEMISTRY 5436
Electronic Structure & Informatics Chem, Spring 2019

Instructor: Dr. James J. Shepherd
Office: E 435 Chemistry Building
Email: james-shepherd@uiowa.edu

Course: CHEM 5436, 3 Credit Hours
Classroom: 9:30A - 10:45A TTh 214 BHC

Office Hours:

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<th>Individual</th>
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| Dr. James Shepherd  | E435 CB  | First four weeks (until 2/8):
|                     |          | Mon 4:30pm to 5:30pm
|                     |          | Weds 2pm to 3pm
|                     |          | or by appointment
|                     |          | Check ICON for all rearrangements and cancellations. Subsequent times to be announced.

Texts:

Course Description:
This course aims to introduce students from both theoretical and experimental backgrounds to the basics of electronic structure theory.

In the first two thirds of the course, students will be guided through the course textbook through a series of short lectures, reading, and discussions. Emphasis will be placed on developing a proficiency in the concepts of electronic structure including density functional theory. I have designed this course such that students will not require a strong mathematical/computational background to succeed in the course.

The final third consists of instructed project work and literature review presentations where students relate the course material to their own field of research. Students will learn how to design a sound computation study relevant to their own background. Primary literature will be used throughout.

The course is intended primarily for chemistry, biochemistry, environmental science, and chemical and biochemical engineering majors. The course requires limited use of differential and integral calculus and skill in mathematical problem solving. This course will count as a Physical Chemistry Proficiency for the Chemistry graduate program.
This course is challenging predominantly because it requires you to interpret diagrams and mathematical expressions in varying contexts to extract new concepts that you have not seen before. In practice, you do this almost every day, but it’s rare to be asked to do this explicitly in a classroom/coursework setting. Reading out information from abstract representations is an information processing skill rather than one of technical/mathematical fluency and must be practiced. We have taken care in this course to separate practicing the process skill from the technical one. Our goal through this course will be to facilitate the learning of information processing and other process skills which will allow you to succeed in class, in the homeworks/exams of this course, and in your future career.

**Course special policies, attendance:** Classroom attendance is extremely important for this class and is your most efficient route to learn the material. This is reflected in the grading structure for this course.

**Course Organization:**
This course has been designed and organized to help you learn physical chemistry, but no course or instructor can learn for you. **Learning is something only you can do.**

Lectures will be conducted in a guided inquiry format. Virtually all of the activities in class will involve teamwork. Part of your responsibility for this course is to assist the other members of your group (and the entire class) in understanding the material.

Classes will take the form of activities centered around worksheets. It is intended that the worksheets guide participation, rather than are an exercise to be completed perfectly. The key is to turn up and try to do what you can.

Homework will consist almost exclusively of reading from the course textbook and associated problem sets. The reading is very important for this course. We will discuss in our first lesson strategies for how to balance your learning outside and inside the classroom.

There will be no examinations for this course. Instead, grading will be based on classroom participation, homework, and project assignments.

**Grading & Grade scale:**

For those students aiming for a B/B+ grade or above:
- You are expected to participate in every class and complete every homework.

For those students aiming for a A-/A grade, in addition to the standard set forward by the statement above:
- You are expected to participate in every class and complete every homework.
- And you are expected to obtain partial or complete mastery of the learning objectives for this course.

Grades will be determined by classroom attendance, activities, homeworks, performance on participation rubrics, and a project. **We believe the variety of assessment methods will**
improve your ability to learn in this course. Final grades will include +/- grades. Those grades will not necessarily be evenly split among the three categories. The College and EPC has recommended that the A+ grade be omitted altogether.

Grades will be earned in approximately the following distributions.

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<tr>
<th>Category</th>
<th>Percentage</th>
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<tbody>
<tr>
<td>Attendance, class participation, minute paper, homework, quizzes</td>
<td>~75%</td>
</tr>
<tr>
<td>Project work</td>
<td>~25%</td>
</tr>
</tbody>
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90% – 100% A
80% – 89%  B
70% – 79%   C
60% – 69%   D
< 60%      F

Expectations for grades are based on degree of mastery of course content. Students may vary in their competency levels on these abilities. Students can expect to acquire these abilities only if they honor all course policies, attend class meetings regularly, complete all assigned work in good faith and on time, and meet all other course expectations. **Students whose achievement is in the indicated ranges will not receive a grade lower than that regardless of the distribution.**

**Attendance Policy:**
Attendance at all lecture sessions is expected. Legitimate reasons for absences are accepted and when possible prior notice of expected absences is requested.

**Prerequisites and Required Background Material:**
The prerequisites for this course include calculus and elementary physics. I will make every effort to introduce important mathematical and physical concepts before we need them, but these elements are an essential part of physical chemistry. Students who have taken CHEM:4432 Physical Chemistry II will find the course straightforward to adapt to.

**Expected Student Workload**
This is a 3 credit hour course.

**Academic Misconduct:**
In addition to the Academic Honesty code offenses detailed by the College, there are course specific expectations regarding Academic Honesty. Academic misconduct may result in a grade reduction and/or other serious penalties, up to and possibly including expulsion from the University of Iowa.

**Examinations:** You are expected to work alone. **Cheating will not be tolerated.** The instructor believes strongly in fairness for all students and objective appraisal of individual performance and understanding of material.

**Problem Sets:** The homework for this course is designed to help you master your knowledge related to the topics covered during lecture. As such, you may work on the homework problems with others or use online resources; however, please be aware that to master the skills needed for this class, practice is required and that to do well on exams you will need to work many of these
problems multiple times without help. Be sure to test your knowledge by doing much of the homework on your own.

**College of Liberal Arts and Sciences (CLAS): Policies and Procedures**

**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](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 correspondence ([Operations Manual, III.15.2](http://uiowa.edu/operations-manual)), k.11).

**Accommodations for Disabilities** - A student seeking academic accommodations should first register with Student Disability Services and then meet privately with Prof. Cole, Haes, and McCurdy to make particular arrangements. See [www.uiowa.edu/~sds/](http://www.uiowa.edu/~sds/) for more information.

**Academic Honesty** - All CLAS students have, in essence, agreed to the College’s [Code of Academic Honesty](http://uiowa.edu/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](http://clas.uiowa.edu/students/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 the 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](http://clas.uiowa.edu/students/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 [Comprehensive Guide on Sexual Harassment](http://uiowa.edu/comprehensive-guide-on-sexual-harassment) 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 [Public Safety website](http://uiowa.edu/public-safety).
**Student Classroom Behavior**

The ability to learn is decreased when students engage in inappropriate classroom behavior, distracting others; such behaviors are a violation of the Code of Student Life. When disruptive activity occurs, an instructor has the authority to determine classroom seating patterns and to request that a student exit the classroom, laboratory, or other instructional area immediately for the remainder of the period. One-day suspensions are reported to Departmental, Collegiate, and Student Services personnel (Office of the Vice President for Student Services and Dean of Students).

**University Examination Policies**

  **Missed exam.** UI policy requires that students be permitted to make up exams missed because of illness, religious obligations, certain University activities, or unavoidable circumstances.

  **Final Examinations.** A student with two final examinations scheduled for the same period or more than three examinations on the same day may file a request for a change of schedule before the published deadline at the Registrar’s Service Center, 17 Calvin Hall, 8-4:30 M-F (384-4300).