4:180 Introduction to Molecular Modeling
Spring 2012

Instructor
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Lecture
9:30-10:45 AM, Tuesday/Thursday. Locations: W241 CB, W244 CB

Office Hour
TBA, or by appointment

Text
Electronic Structure Calculations for Solids and Molecules, Jorge Kohanoff, ©2006 Cambridge University Press. (The text is also available online through the UI Library site.)

Website
http://icon.uiowa.edu

Course Objectives
To develop conceptual understanding of, and practical experience with, electronic structure problems studied in condensed matter physics and theoretical chemistry. We will study various theoretical approaches and computational techniques used in electronic structure calculations starting from basic approximations and including an overview of modern challenges in methodology development. We will also study the pragmatic issue of how quantum mechanical problems are translated into a form solvable by computation. 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.

Course Content
• Dirac notation and matrix mechanics
• Variational principle and perturbation theory
• Structure of the Hamiltonian
• Hartree-Fock theory and quantum chemical methods
• Density functional theory (DFT)
• Atomic pseudopotentials
• Exchange and correlation in DFT
• Simplified approaches to the electronic problem
• Self-consistency: Mixing schemes and minimization techniques

Grading
Problem Sets 25%
In-class computational work and participation 35%
Quizzes 15%
Final project/oral presentation 25%
Final course grades will use ± designation.
Prerequisites and Required Background Material
The co-requisite for this course is 4:132 (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.

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 solution set. 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. Hands-on computational work during class time may be done in small groups, resulting in a single final product, as long as I observe participation from all group members.

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 Student Academic 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 privately with the course instructor to make particular arrangements. See www.uiowa.edu/~sds/ for more information.
Academic Fraud
Plagiarism and any other activities when students present work that is not their own are academic fraud. Academic fraud is a serious matter and is reported to the departmental DEO and to the Associate Dean for Undergraduate Programs and Curriculum. Instructors and DEOs decide on appropriate consequences at the departmental level while the Associate Dean enforces additional consequences at the collegiate level. See the CLASH Academic Fraud section of the Student Academic Handbook.

CLAS Final Examination Policies
Final exams may be offered only during finals week. No exams of any kind are allowed during the last week of classes. Students should not ask their instructor to reschedule a final exam since the College does not permit rescheduling of a final exam once the semester has begun. Questions should be addressed to the Associate Dean for Undergraduate Programs and Curriculum.

Making a Suggestion or a Complaint
Students with a suggestion or complaint should first visit the instructor, then the course supervisor, and then the departmental DEO. Complaints must be made within six months of the incident. See the CLAS Student Academic 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 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 web site.

*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.