Syllabus for CHEM 5660
Introduction to Computational Chemistry
Spring 2010

Instructor: Dr. Angela Wilson

Office Hours: Mondays, 1:00 p.m. – 3:00 p.m.; 5:00 – 6:00 p.m.

Office: Chemistry 205C

Office Phone: (940) 565-4296

E-mail: akwilson@unt.edu

Class times: Mondays, 6:00 – 8:50 p.m.

Class locations: Computational Chemistry Instructional Laboratory (CCIL) and CHEM 352


Assistant: Gbenga Oyedepo; Additional help may be sought in the Computational Chemistry Instructional Laboratory, where computational chemistry graduate students are available to provide assistance whenever CCIL is open.

Office: Chemistry 262

Office Hours: TBA

Office Phone: (940) 565-2948

E-mail: gbengao@gmail.com

COURSE CONTENT
This course provides a “hands-on” approach to the practical application of computers in analyzing and understanding molecular structures and chemical reactions. We will focus on the use of both basic and advanced computational methods. We will learn not only about software that can help us visualize concepts but also about software packages such as Gaussian 03 that serve as an aid to experiment. We will use a variety of computational platforms ranging from PC’s to substantial computer clusters, and will become familiar with the Linux operating system in a multi-user environment.
COURSE GOALS
(1) To become familiar with a variety of computational chemistry techniques, including methods for visualization as well as those used to analyze molecular properties.
(2) To be able to use computational chemistry techniques as an aid to experiment.
(3) To be able to determine which computational approach should be used in various situations.
(4) To become proficient in the use of a variety of computer platforms in chemistry studies.

COURSE ASSIGNMENTS

READING ASSIGNMENTS
Significant amounts of reading will be required from your text, as well as from several other sources. These additional sources include texts (sources: library, online), program documentation (sources: on pertinent computer systems), documentation specific to the operating system and computers we will be using (sources: hand-outs, online, man pages on pertinent computer systems), and journal articles (sources: internet, library). It is important that you come to class prepared to work. It is essential that you keep up with the reading. You will be learning a large amount of terminology and acronyms throughout the semester and many new concepts. Read the assigned pages PRIOR to class and be prepared to discuss the material you read.

COURSE GRADING

GRADING FOR CHEM 5660 (TENTATIVE*)

<table>
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<th>Assignment</th>
<th>Points</th>
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<tr>
<td>Project</td>
<td>300 pts</td>
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<tr>
<td>Topic Presentation</td>
<td>100 pts</td>
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<tr>
<td>Assignments/Project Checks</td>
<td>100 pts</td>
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<tr>
<td>Mid-Term Exam</td>
<td>200 pts</td>
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<td>Final Exam</td>
<td>300 pts</td>
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<tr>
<td><strong>TOTAL POINTS FOR CHEM 5660</strong></td>
<td><strong>1000 pts</strong></td>
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FINAL GRADES WILL BE BASED UPON:
A = 90-100%
B = 80-89%
C = 70-79%
D = 60-69%
F = Below 60%

PROJECT (WEDNESDAY, MAY 5, 3:00 p.m.)
At the mid-point of the semester, you will begin a long-term project that will be developed (in consultation with Dr. Wilson) which will enable you to explore a scientific problem of interest to you. You will use the skills that you develop and methods that you become familiar with during the early part of the semester in this project. Thus, it is essential that you master the skills and methods early in the semester! Once you begin this phase of the course, you will be asked
periodically for updates on your project progress (which will be counted as part of your overall project report). Be prepared to provide these. Points will be deducted for lack of progress on projects. Zero points will be awarded to projects that do not begin until the last few weeks of the semester. Hand-outs will be given (at a later date) that describe the project.

**TOPIC PRESENTATION (April 19):**
During the course of the semester, we do not have time to cover all aspects of computational chemistry. This presentation will provide you with the chance to present a topic of interest to you that will not be covered otherwise during the course.

**MID-TERM EXAM (March 8) and FINAL EXAM (May 6)**
These exams will be on paper and/or on computer (i.e. “Show how you would run, compute, set up a calculation for, . . . “). They will cover the reading assignments, lectures, our discussions, and exercises.

**HOMEWORK ASSIGNMENTS (due dates provided with assignments)**
Throughout the early part of the course, a series of homework exercises will be assigned. It is very important to keep up weekly in the class. For that reason, the above grading scheme is “tentative”. Project checks may be given (which entail unannounced quizzes) and additional homework assignments may be given, if necessary.

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**Attendance Policy**
Because this course is a hands-on training course, an attendance policy will be enforced. Any student with unexcused absences during the first three weeks of the course or who misses a total of 10% of the semester classes will receive an instructor withdrawal (WF) or an F in the course.

Excused absences include: conference participation (but notification is required PRIOR to the absence), death in the family, and illness (a note from a physician is required).

Material/instructions will NOT be repeated by the instructor for those with unexcused absences. Assignments and exams can not be made-up.

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**TECHNIQUE:**
Good laboratory technique is just as important in theoretical (computational) chemistry as it is in the traditional chemistry laboratory. However, “good technique” is defined a bit differently. “Good technique” entails: (1) backing up data; (2) keeping good track of your results; (3) using resources wisely; (4) being familiar with and following all guidelines for each computer platform you use; (5) removing your files at the end of the semester; and (6) understanding the types of computer systems on which you are running calculations. Further details for each of these follow:

(1) *Backing up data* – Some of the calculations you will do may take up large amounts of computer time. You should always be in the practice of backing up your data. You will need to back up your data on your own PC, on CD’s, on flash drives, external drives, etc.
(2) Keeping good track of your results – You will be running many calculations this semester. Be sure to keep good track of them. Naming directories and subdirectories according to the program, method, or system you are running will be useful, as well as a **well-documented lab notebook** (WHICH YOU WILL TURN IN WITH YOUR PROJECT AT THE END OF THE SEMESTER). Be sure that you record which computer you used for each calculation.

(3) Using resources wisely – First, each calculation will generate a large amount of output. **DO NOT PRINT OUT ALL OF THE OUTPUT UNLESS ABSOLUTELY NECESSARY!** (And, rarely will it be necessary!) Second, use your resources wisely. Both the computer cluster and the SGI Altix are shared resources. On the computer cluster, you will be sharing the resources with your classmates. On the SGI Altix, you will be sharing the computer with users throughout the U.S. and, as a class, we only have a certain amount of time on the system which we will be sharing with one another. It is very simple to forget to cancel a job or make other similar mistakes which could result in using all of these resources. Be particularly careful when you are using this system! If in doubt about anything, please contact Dr. Wilson or Ben FIRST. (Any misuse of the system will result in a reduction in the overall semester grade as well as termination of resource access.)

(4) Being familiar with and follow all guidelines for each computer platform you use – First and foremost, **DO NOT SHARE YOUR PASSWORD FOR THE NCSA SGI ALTIX OR UNT CHEMISTRY SYSTEMS WITH ANYONE UNDER ANY CIRCUMSTANCES!** Second, these systems have batch queues to which you must submit your calculations. Always use the batch system unless Dr. Wilson or Gbenga tell you otherwise. Failure to comply with specific computer platform guidelines or sharing your password will result in failure of course!

(5) Removing your files at the end of the semester – If you have done (2) throughout the semester, you will be able to complete this task quite easily! However, if you have not kept track of where all your files reside, this task will become quite tedious!

(6) Understanding the types of computer systems on which you are running calculations. While you are not expected to become an expert about the detailed configuration for every computer system that you use, you should have basic knowledge about each platform. For example, what operating system are you using? How many processors does the system have? How much memory and disk space is available on the system? Is it a shared-memory system, or, what are the per-node limits? How fast are the processors? Some of the issues are going to be very important to you when you have to make decisions about resources you need to run calculations.

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**COURSE WEB PAGE:**

Supplemental course information may be found at:

http://www.chem.unt.edu/~akwilson/chem5660/chem5660.html
NOTE: This department believes in reasonably accommodating individuals with disabilities and complies with the university policy established under Section 504 of the Rehabilitation Act of 1973 and the Americans with Disabilities Act (1990) to provide for equal access and opportunity. Please communicate with your professor as to your specific needs so appropriate arrangements can be made through the department and/or the Office of Disability Accommodation (Room 318A, University Union, (940) 565-4323).

Drop deadline: Tuesday, March 25.

Holiday: No class on Tuesday, March 18 (Spring break).
### Tentative Class Outline:

<table>
<thead>
<tr>
<th>DATE</th>
<th>TOPICS</th>
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| JAN. 25 | Introduction to computational chemistry  
          | Introduction to computational chemistry methods  
          | Introduction to Linux and vi; security issues |
| FEB. 1  | Spartan  
          | GaussView |
| FEB. 8  | Molecular mechanics  
          | z-matrices; ghost atoms  
          | Introduction to Gaussian 03; input and understanding output |
| FEB. 15 | Semi-empirical methods  
          | Geometry optimization vs. single-point  
          | Visualization freeware  
          | Frequency calculations  
          | FTPing data; protecting data |
| FEB. 22 | *Ab initio* methods; basis sets |
| MARCH 1 | Electron correlation methods  
          | Mid-term review |
| MARCH 8 | **MID-TERM EXAM**  
          | Electron correlation methods |
| MARCH 15| SPRING BREAK |
| MARCH 22| Advanced options  
          | Additional properties  
          | Selecting an appropriate model |
| MARCH 29| Density functional theory |
| APRIL 5 | Advanced topics |
| APRIL 12| Advanced topics |
| APRIL 19| Topic presentation |
| APRIL 26| Advanced topics |
| MAY 3  | Advanced topics |
| MAY 5  | Project due |
| MAY 10 | **FINAL EXAM** |