

Course Syllabus

Course Information

(course number, course title, term, any specific section title)

Special Topics in Physical Chemistry - CHEM-6V19-001 – 2009S

TR 10:00-11:15 BE3.102

Professor Contact Information

(Professor's name, phone number, email, office location, office hours, other information)

Dr. Steven O. Nielsen, 972-883-5323, steven.nielsen@utdallas.edu, BE2.516.

Office hours: Please feel free to stop by whenever you have a question.

Course Pre-requisites, Co-requisites, and/or Other Restrictions

(including required prior knowledge or skills)

Prerequisite: CHEM 5314 or consent of instructor.

Course Description

Subject matter will vary and the course may be repeated for credit. Examples of topics include spectroscopy, quantum mechanics, computational chemistry, and surface chemistry.

Student Learning Objectives/Outcomes

Objectives: The student will become familiar with the physical basis for molecular modeling and will learn to apply some of the currently available modeling packages to problems of interest in chemistry. The emphasis will be on utility: How well do particular techniques reproduce reality and how much insight do they provide about chemistry?

Outcomes: To this end, students will be able to

1. Explain the strengths and weaknesses and the approximations inherent to different quantum chemical computational methods;
 2. Deduce molecular properties (e.g. structure, reactivity) from computational modeling data; and
 3. Interpret which computational method or combination of methods is appropriate for a given chemistry problem and propose an approach to arrive at a solution.
-

Required Textbooks and Materials

Modern quantum chemistry, introduction to advanced electronic structure theory by Attila Szabo and Neil S. Ostlund; published by Dover

possibly a statistical mechanics/classical simulation book later in the semester

<http://www.utdallas.edu/~son051000/chem6V19.html>

Suggested Course Materials

I will provide suggestions as the semester progresses.

Assignments & Academic Calendar

(Topics, Reading Assignments, Due Dates, Exam Dates)

The following is a rough outline – we may go faster or slower through the material.

| | | |
|---------|--------|--------------------------------------|
| Jan. 13 | 15 | quantum |
| 20 | 22 | quantum |
| 27 | 29 | quantum |
| Feb. 3 | 5 | quantum |
| 10 | 12 | quantum |
| 17 | 19 | quantum |
| 24 | 26 | quantum |
| Mar. 3 | 5 | classical |
| 10 | 12 | classical (Spring Break March 16-21) |
| 24 | 26 | classical |
| 31 | Apr. 2 | classical |
| 7 | 9 | classical |
| 14 | 16 | classical |
| 21 | 23 | classical |
| 28 | 30 | classical |

Grading Policy

(including percentages for assignments, grade scale, etc.)

The course grade will be based on homework (50%) and two papers/presentations on topics chosen/approved by the instructor (50%).

Course & Instructor Policies

(make-up exams, extra credit, late work, special assignments, class attendance, classroom citizenship, etc.)

There will be no makeup exams given. If you have an acceptable, documented reason for missing a term test (e.g. documented illness), you will be allowed to replace the missed term test with your score on the final. Otherwise, you will receive a zero. The final exam must be taken, will be comprehensive and cannot be replaced by any other grade. Homework turned in after the answers are posted online will not receive any credit.

Field Trip Policies

Off-campus Instruction and Course Activities

Off-campus, out-of-state, and foreign instruction and activities are subject to state law and University policies and procedures regarding travel and risk-related activities. Information regarding these rules and regulations may be found at the website address http://www.utdallas.edu/BusinessAffairs/Travel_Risk_Activities.htm. Additional information is available from the office of the school dean. Below is a description of any travel and/or risk-related activity associated with this course.

Student Conduct & Discipline

The University of Texas System and The University of Texas at Dallas have rules and regulations for the orderly and efficient conduct of their business. It is the responsibility of each student and each student organization to be knowledgeable about the rules and regulations which govern student conduct and activities. General information on student conduct and discipline is contained in the UTD publication, *A to Z Guide*, which is provided to all registered students each academic year.

The University of Texas at Dallas administers student discipline within the procedures of recognized and established due process. Procedures are defined and described in the *Rules and Regulations, Board of Regents, The University of Texas System, Part I, Chapter VI, Section 3*, and in Title V, Rules on Student Services and Activities of the university's *Handbook of Operating Procedures*. Copies of these rules and regulations are available to students in the Office of the Dean of Students, where staff members are available to assist students in interpreting the rules and regulations (SU 1.602, 972/883-6391).

A student at the university neither loses the rights nor escapes the responsibilities of citizenship. He or she is expected to obey federal, state, and local laws as well as the Regents' Rules, university regulations, and administrative rules. Students are subject to discipline for violating the standards of conduct whether such conduct takes place on or off campus, or whether civil or criminal penalties are also imposed for such conduct.

Academic Integrity

The faculty expects from its students a high level of responsibility and academic honesty. Because the value of an academic degree depends upon the absolute integrity of the work done by the student for that degree, it is imperative that a student demonstrate a high standard of individual honor in his or her scholastic work.

Scholastic dishonesty includes, but is not limited to, statements, acts or omissions related to applications for enrollment or the award of a degree, and/or the submission as one's own work or material that is not one's own. As a general rule, scholastic dishonesty involves one of the following acts: cheating, plagiarism, collusion and/or falsifying academic records. Students suspected of academic dishonesty are subject to disciplinary proceedings.

Plagiarism, especially from the web, from portions of papers for other classes, and from any other source is unacceptable and will be dealt with under the university's policy on plagiarism (see general catalog for details). This course will use the resources of turnitin.com, which searches the web for possible plagiarism and is over 90% effective.

Email Use

The University of Texas at Dallas recognizes the value and efficiency of communication between faculty/staff and students through electronic mail. At the same time, email raises some issues concerning security and the identity of each individual in an email exchange. The university encourages all official student email correspondence be sent only to a student's U.T. Dallas email address and that faculty and staff consider email from students official only if it originates from a UTD student account. This allows the university to maintain a high degree of confidence in the identity of all individual corresponding and the security of the transmitted information. UTD furnishes each student with a free email account that is to be used in all communication with university personnel. The Department of Information Resources at U.T. Dallas provides a method for students to have their U.T. Dallas mail forwarded to other accounts.

Withdrawal from Class

The administration of this institution has set deadlines for withdrawal of any college-level courses. These dates and times are published in that semester's course catalog. Administration procedures must be followed. It is the student's responsibility to handle withdrawal requirements from any class. In other words, I cannot drop or withdraw any student. You must do the proper paperwork to ensure that you will not receive a final grade of "F" in a course if you choose not to attend the class once you are enrolled.

Student Grievance Procedures

Procedures for student grievances are found in Title V, Rules on Student Services and Activities, of the university's *Handbook of Operating Procedures*.

In attempting to resolve any student grievance regarding grades, evaluations, or other fulfillments of academic responsibility, it is the obligation of the student first to make a serious effort to resolve the matter with the instructor, supervisor, administrator, or committee with whom the grievance originates (hereafter called "the respondent"). Individual faculty members retain primary responsibility for assigning grades and evaluations. If the matter cannot be resolved at that level, the grievance must be submitted in writing to the respondent with a copy of the respondent's School Dean. If the matter is not resolved by the written response provided by the respondent, the student may submit a written appeal to the School Dean. If the grievance is not resolved by the School Dean's decision, the student may make a written appeal to the Dean of Graduate or Undergraduate Education, and the dean will appoint and convene an Academic Appeals Panel. The decision of the Academic Appeals Panel is final. The results of the academic appeals process will be distributed to all involved parties.

Copies of these rules and regulations are available to students in the Office of the Dean of Students, where staff members are available to assist students in interpreting the rules and regulations.

Incomplete Grade Policy

As per university policy, incomplete grades will be granted only for work unavoidably missed at the semester's end and only if 70% of the course work has been completed. An incomplete grade must be resolved within eight (8) weeks from the first day of the subsequent long semester. If the required work to complete the course and to remove the incomplete grade is not submitted by the specified deadline, the incomplete grade is changed automatically to a grade of **F**.

Disability Services

The goal of Disability Services is to provide students with disabilities educational opportunities equal to those of their non-disabled peers. Disability Services is located in room 1.610 in the Student Union. Office hours are Monday and Thursday, 8:30 a.m. to 6:30 p.m.; Tuesday and Wednesday, 8:30 a.m. to 7:30 p.m.; and Friday, 8:30 a.m. to 5:30 p.m.

The contact information for the Office of Disability Services is:
The University of Texas at Dallas, SU 22
PO Box 830688
Richardson, Texas 75083-0688
(972) 883-2098 (voice or TTY)

Essentially, the law requires that colleges and universities make those reasonable adjustments necessary to eliminate discrimination on the basis of disability. For example, it may be necessary to remove classroom prohibitions against tape recorders or animals (in the case of dog guides) for students who are blind. Occasionally an assignment requirement may be substituted (for example, a research paper versus an oral presentation for a student who is hearing impaired). Classes

enrolled students with mobility impairments may have to be rescheduled in accessible facilities. The college or university may need to provide special services such as registration, note-taking, or mobility assistance.

It is the student's responsibility to notify his or her professors of the need for such an accommodation. Disability Services provides students with letters to present to faculty members to verify that the student has a disability and needs accommodations. Individuals requiring special accommodation should contact the professor after class or during office hours.

Religious Holy Days

The University of Texas at Dallas will excuse a student from class or other required activities for the travel to and observance of a religious holy day for a religion whose places of worship are exempt from property tax under Section 11.20, Tax Code, Texas Code Annotated.

The student is encouraged to notify the instructor or activity sponsor as soon as possible regarding the absence, preferably in advance of the assignment. The student, so excused, will be allowed to take the exam or complete the assignment within a reasonable time after the absence: a period equal to the length of the absence, up to a maximum of one week. A student who notifies the instructor and completes any missed exam or assignment may not be penalized for the absence. A student who fails to complete the exam or assignment within the prescribed period may receive a failing grade for that exam or assignment.

If a student or an instructor disagrees about the nature of the absence [i.e., for the purpose of observing a religious holy day] or if there is similar disagreement about whether the student has been given a reasonable time to complete any missed assignments or examinations, either the student or the instructor may request a ruling from the chief executive officer of the institution, or his or her designee. The chief executive officer or designee must take into account the legislative intent of TEC 51.911(b), and the student and instructor will abide by the decision of the chief executive officer or designee.

These descriptions and timelines are subject to change at the discretion of the Professor.