CHEM 6343
Advanced Computational Chemistry

Class location:	TBD
Lectures, time and location:	TBD
Lab times and location:	TBD
Instructor:	Elfi Kraka, 231 FOSC, ext 8-2480, ekraka@smu.edu http://smu.edu/catco/
Office Hours:	By appointment
Units:	3
Grading:	ABC Letter Grade
Class number	

1. Rationale:

Besides the normal lab experiments traditionally expected, modern chemists/biochemists perform "experiments" on the computer by calculating the outcome of a chemical reaction. This *in silicio* chemistry has become an integral part of the education in chemistry and the present course will provide an introduction into this new field by addressing a general audience of chemists/biochemists and students from neighboring fields. Starting from the description of atomic and molecular electronic structure, and then discussing the elementary processes of bond breaking and forming, the course leads to the calculation of typical chemical reactions in a hands-on fashion. Major quantum chemical packages will be used for this purpose.

2. Course Recommendations:

The course is designed for all graduate students from chemistry, biochemistry, medicinal chemistry, biology, and physics who are interested in physical chemistry and/or to learn how to solve chemical problems on the computer. Since the course addresses a broad audience, it is designed as an interdisciplinary course taking care of the special needs of students with different background. instructor. The course does not require detailed knowledge in mathematics or quantum chemistry.

3. Texts:

- Textbook: P.W. Atkins and R.S. Friedman, "Molecular Quantum Mechanics", Third Edition, Oxford University Press, New York, 1997.
- Handouts and notes for the computer labs.

4. Course Aims and Objectives:

The course will discuss the basic principles of quantum mechanics, which are necessary to understand the properties of atoms and molecules and their chemical reaction. A variety of different methods for the calculation of molecular properties will be systematically discussed,

ranging from very accurate methods for small molecules to less accurate methods for large molecules. The material will be presented in a form that a chemist or biochemist can follow without getting lost in mathematical derivations and difficult equations.
The methods discussed will be applied in the computer labs to solve typical chemical problems, which are taken from the actual research in the theoretical chemistry group. In this way the student gets a realistic training how to use computational tools in his/her studies or later career in academia or private industry.

Specific Learning Objectives:
By the end of this course, students:

will have a conceptual understanding of the laws of quantum mechanics necessary for the description of atoms and molecules and their chemical reaction;
will be able to choose the appropriate method (in terms of applicability, accuracy, and economy) for the calculation of a given chemical problem;
will be able to perform, understand, and interpret the results of the calculations and bring them in a publication ready form.

General Education Learning outcomes:
3 III. Science and Technology

- 3.1 Students demonstrate basic facility with the methods and approaches of scientific inquiry and problem solving.
- 3.2 Students explain how the concepts and findings of science in general, or of particular sciences, shape our world.

5. Course Outline:

In 14 chapters, the course leads from early quantum theory to modern ab initio calculations:

1. Early Quantum Theory: historical overview; influence of physics on Theoretical Chemistry; blackbody radiation; photoelectric effect; Bohr and the H atom; de Broglie wavelength; Heisenberg uncertainty principle.
2. The wave equation: differential equations; separation of variables
3. The Schrödinger equation and simple applications such as the particle in the box
4. Basic Quantum Mechanics: state of a system; operators and observables; postulates and general principles of quantum mechanics.
5. The Harmonic oscillator: diatomic molecules; solution of the harmonic oscillator problem; quantum mechanical tunneling
6. From one to three dimensions: particle in the 3-dimensional box; the rigid rotator; the hydrogen atom; quantum numbers; orbitals.
7. Approximated methods: independent particle approximation; variational method; perturbation theory.
8. Calculation of atoms: application of variational method and perturbation theory to the He atom; Hartree-Fock calculation of the He atom; electron spin and Pauli principle; antisymmetric wave functions and Slater determinants; singlet and triplet wave functions; atomic term symbols.
9. Calculation of molecules: Valence bond theory of H_2; chemical bonding; Molecular Orbital theory, theory of H_2^+ and H_2; improvement of valence bond theory; generalized valence bond; configuration interaction with single and double excitations.

10. Hartree-Fock theory: Fock operator; Hartree-Fock equations; linear combination of atomic orbital-ansatz; Roothaan-Hall equations; self-consistent field approach.
11. Ab initio theory: basis sets; restricted and unrestricted Hartree-Fock; electron correlation; many body perturbation theory, coupled cluster theory, multi configuration self-consistent field theory.
12. Semi-empirical methods: π-methods; Valence electron methods: extended Hückel; Neglect of Differential Overlap methods: Austin Model 1, Parameter Model 3; use of semi-empirical methods.
13. Density Functional Theory: basic idea, homogeneous electron gas, Coulomb hole, exchange hole, use of Density Functional Theory in quantum chemistry, Kohn-Sham equations, exchange functionals, correlation functionals, hybrid functionals.
14. Mixed methods, like the combination of quantum chemical methods and molecular mechanics (QM/MM) for the description of biochemical problems, for example the interaction of a drug and a receptor.
15. Simulation of macroscopic properties. Basic terms from statistical mechanics, Concept of the ensemble, standard thermodynamic functions expressed in partition functions, Monte Carlo (MC) methods, MD simulation methods.

15 mandatory computer labs complement the lectures. In these labs the students learn how to solve chemical problems by means of ab-initio theory and Density Functional Theory calculations. Examples are taken from current research within theoretical chemistry (e.g. problems from atmospheric chemistry, anti-cancer chemistry, etc.). It will be trained how to calculate molecular properties as energy, geometry, vibrational frequencies, NMR chemical shifts, dipole moments. Advanced topics are modification and design of basis sets, calculation of reaction rates by means of variational transition state theory, reaction path following, and the description of a biochemical problem with QM/MM. The emphasis will be on using the best possible method and basis set (according to accuracy and economy) for a given problem. It will be discussed, how to derive chemical important information from the numbers produced, how to bring the results in a form ready for publication.

6. Student Responsibilities:

We are planning to have a quiz after every second chapter. Therefore, it is recommended that each student actively participate in the lectures. The student has to hand in a lab report for each computer lab along the lines described in the lab instructions. Each quiz and lab report will count toward the final grade. Questions regarding grades should be brought to the instructor's attention within one week after receiving back the exam.

7. Final Examination: Weak 18, day and time TBD

8. Grading Procedures:

Final grades will be calculated according to the following scheme:

Final exam	40%
Quizzes	30%
Lab reports	30%

Grading Table		
	A	100 – 90 %
	B	89 – 80 %
	C	79 – 70 %
	D	69 - 60 %
	F	59% and below

9. Statement of Honor Code:
All SMU Dedman College students are bound by the honor code. The applicable section of the code reads: "All academic work undertaken at the University shall be subject to the guidelines of the Honor Code. Any giving or receiving of aid on academic work submitted for evaluation, without the express consent of the instructor, or the toleration of such action shall constitute a breach of the Honor Code." A violation of the Code can result in an F for the course and an Honor Code Violation recorded on a student's transcript. Academic dishonesty includes plagiarism, cheating, academic sabotage, facilitating academic dishonesty and fabrication. Plagiarism is prohibited in all papers, projects, take-home exams or any other assignments in which the student submits another's work as being his or her own. Cheating is defined as intentionally using or attempting to use unauthorized materials, information or study aids in any academic exercise. Academic sabotage is defined as intentionally taking any action, which negatively affects the academic work of another student. Facilitating academic dishonesty is defined as intentionally or knowingly helping or attempting to help another to violate any provision of the Honor Code. Fabrication is defined as intentional and unauthorized falsification or invention of any information or citation in an academic exercise.

10. Disability Accommodations:
Students needing academic accommodations for a disability must first contact Ms. Rebecca Marin, Director, Services for Students with Disabilities (214-768-4557) to verify the disability and establish eligibility for accommodations. They should then schedule an appointment with the professor to make appropriate arrangements.

11. Religious Observance:
Religiously observant students wishing to be absent on holidays that require missing class should notify their professors in writing at the beginning of the semester, and should discuss with them, in advance, acceptable ways of making up any work missed because of the absence.

12. Excused Absences for University Extracurricular Activities:
Students participating in an officially sanctioned, scheduled University extracurricular activity should be given the opportunity to make up class assignments or other graded assignments missed as a result of their participation. It is the responsibility of the student to make arrangements with the instructor prior to any missed scheduled examination or other missed assignment for making up the work.

13. Assessment:
In accordance with University regulations copies of student work may be retained to asses how the learning objectives of the course are being met.

14. Course Schedule:
Will be discussed in the first meeting worked out to accommodate best to the student needs.