CHEM 6115
Theory of the Chemical Bond, Spring/2010

Lectures, time and location:	TBD
Course period and start:	3rd period, starting April 1st
Instructor:	Dieter Cremer, 325 FOSC, ext 8-1300, dcremer@smu.edu http://smu.edu/catco/
Office Hours:	By appointment
Units:	1
Grading:	ABC Letter Grade

1. Rationale:
Chemical bonding is at the heart of Chemistry. It is the physical reason why about hundred naturally occurring elements form more than 50 million known chemical compounds, which make up our world. Hence, any chemist must know about the essence of chemical bonding, that this is a quantum mechanical phenomenon, and how bonding can be described utilizing either orbitals, the electron density, or the quantum mechanical interaction energies between electrons and nuclei. Chemists have to know the different forms of chemical bonding and how bond properties determine the structure, stability, and reactivity of chemical compounds.

2. Course Recommendations
The course is important for all students from chemistry, biochemistry, biology, and physics who have to know about the forces that keep atoms and molecules together in chemical compounds, and in addition determine their structure, stability, and reactivity. Special care will be taken that students with different background can follow the course. There is no need to have already knowledge in quantum mechanics. Mathematics and physical chemistry will play a minor role. However there will be ample examples of different bonding types from current chemistry.

3. Texts
• Handouts.

4. Course Aims and Objectives:
The course will discuss the basic principles of chemical bonding, which have to be known to understand why atoms clutch together to form chemical compounds. Each student will learn about basic quantum mechanical forces, elementary molecular orbital theory, and some principles of density theory. The difference between model and measurable quantities will be amply discussed in the case of bond properties. A variety of different bond types will be known by the end of the course so that the student can identify these bond types in a given molecule, can relate them to structural, stability, and reactivity features, and predict a number of properties for the molecule in question. General aim of the course is a better understanding of chemistry rather than gaining specific knowledge in quantum mechanics, mathematics, or physical chemistry. Therefore a large number of chemical problems will be discussed within the course and the homework.

Specific Learning Objectives:

By the end of this course, students

will have a conceptual understanding of chemical bonding and the quantum mechanical forces that lead to bonding;

will be able to distinguish between different types of bonding;

will be able to relate bond properties to the type of bonding;

will be able to understand the relationship between bonding, structure, stability, and reactivity

General Education Learning outcomes:

1. Students have to demonstrate basic facility with the methods and approaches of scientific inquiry and problem solving.

2. Students have to explain how the concepts and findings of science in general, or of particular sciences, shape our world.

5. Course Outline

In 11 chapters, the course will develop essential features of modern bonding theory:

1) Characterization of chemical bonds: typical bond dissociation energies, bond lengths, bond polarities, and other bond properties; examples of unusual bonds; bent and strained bonds, sigma, pi, and delta bonds, partial bonds, localized and delocalized bonds

2) Can one observe chemical bonds? Atoms in molecules; concept of the chemical bond; bonding models: classical models; orbital-description of bonding; electron density description of bonding, quantum chemical description of the bond

3) Bond strength and how to determine it: bond energy and bond dissociation energy, bond length, bond density, bond stretching frequency, bond stretching force constant, bond polarizability, intrinsic bond dissociation energy, bond order

4) Covalent versus ionic bonding: description of bonding in diatomic and polyatomic molecules, single and multiple bonding, bond polarity and electronegativity, ionic character of a bond, ionic bonding and bond strength

5) n-Electron Bonds: 1-electron- and 3-electron-bonds; 3-center-2-electron and 3-center-4-electron bonds, donor-acceptor bonding, dative bond (semipolar bond), charge transfer, electron-deficient bonds, classical and non-classical bonding

6) Delocalized and localized bonding: Bonding and the structure of molecules; bonding and overlap, hybridization model, conjugation, aromatic bond; hyperconjugation, anomeric effect, through-space and through-bond interactions

7) Hypervalent bonding and bonding in transition metal complexes: quadruple, quintuple, and sextuple bonding, relativistic effects on bonding

8) Dynamic models of the chemical bond: breaking and forming of a bond, the role of molecular vibrations; When does a bond stop to be a bond, when does it start to be bond? What happens in a chemical reaction at the transition state? Mechanism of dissociation reactions

9) Metallic Bonding: from bonding in linear conjugated molecules to bonding in solids, band structure theory, k-space, dispersion of the band, Peierls distortion, conductor, semiconductor, insulator properties; bonding, ductility, and hardness

10) Noncovalent Interactions: interactions in van der Waals molecules, electrostatic, inductive, dispersion, and exchange repulsion forces; H-bonding, agostic and anagostic bonding, π-stacking, Casimir forces

11) Bond peculiarities: bond fluctuations, bond-pseudorotation; Which bonds have the highest bond orders? Which are the strongest? Extreme bond lengths; open questions in modern bond theory

6. Student Responsibilities:
a) Students have to attend each lecture and actively participate in them.
b) Students have to hand in homework for each hour and present their reading tasks in short oral or written summaries.
c) In addition to the final exam, there will be 4 quizzes, one after each second or third chapter.
Students have to pass quizzes and exams to pass the course.
Questions regarding grades should be brought to the instructor's attention within 2 days after receiving back the quiz or the exam.

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

8. Grading Procedures:
Final grades will be calculated according to the following scheme:

Final exam	30%
Quizzes	30%
Homework	30%
Special assignments	10%

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 assess how the learning objectives of the course are being met.

14. Course Schedule
Will be discussed in the first meeting and adjusted, as far as possible, to the student needs.