CHEM 6341
Models and Concepts in Chemistry, Spring term

Class location:	TBD
Lectures, time and location:	TBD
Lab times and location:	TBD
Instructor:	Dieter Cremer, 325 FOSC, ext 8-1300, dcremer@smu.edu http://smu.edu/catco/
Office Hours:	By appointment
Units:	3
Grading:	ABC Letter Grade
Class number	TBD

1. Rationale:
In chemistry, every year 2 million new chemical facts are added to what is known since decades and centuries. No chemist can memorize just a fraction of this data. Nevertheless, chemists must be able to adjust their knowledge to all new chemical observations. This is effectively done by a series of models and concepts, which summarizes myriads of data in a simple way.
The course focuses on a general understanding of chemistry in terms of models and concepts that describe structure, stability, reactivity and other properties of molecules in a simple, yet very effective way. The concept of electronegativity, the concept of the chemcial bond, molecular orbital theory, orbital symmetry, the Mulliken-Walsh model, the concept of the potential energy surface, the Jahn-Teller effects, conjugation and delocalization models, the Hückel and Möbius (anti)aromaticity concepts, through-space and through-bond interaction models, the concept of the hydrogen bond, the Woodward-Hoffman rules, the Evans-Dewar-Zimmermann rules, and the isolobal concept will be discussed among other topics. Many chemical problems from organic chemistry, inorganic chemistry, transition metal chemistry, and biochemistry will be presented and the applicability of the various models and concepts as well as their limitations will be demonstrated.

2. Course Recommendations:
The course is designed to reach all graduate students in Chemistry and related disciplines. It does not require any mathematical or quantum mechanical knowledge.

3. Texts:
Presently, there exists no textbook that reflects the contents of the course. Parts of the course have been taken from a) T.A. Albright, J.K. Burdett, M.H. Whangbo, Orbital Interactions in Chemistry, Wiley and b) Y. Jean, F. Volatron, J. K. Burdett, An Introduction to Molecular Orbitals. One of these books may be bought, however this is not absolutely necessary for following the course since a compendium of 300 pages will be handed out, which summarizes

the course content. Please note that just reading of this compendium cannot replace attendance to the lectures and exercises.

4. Course Aims and Objectives:

The course pursues three general goals

1) Clarification of well-known terms, which have their hidden problematic character although most chemists think that he/she uses the terms in the right way (differences between structure and geometry, electron delocalization and bond delocalization, etc. are well-known examples). In this connection, the course aims at providing a better insight into the models and concepts used on a daily basis in chemistry.

2) Many students are under the impression that inorganic, organic or biochemistry are different fields of chemistry that have not so much in common. In the course, it is shown that from a conceptual point of view (e.g. based on atomic and molecular orbital models) there is not much difference between the various disciplines of chemistry. The course aims at drawing connections between the different fields of chemistry to provide a unified picture of the chemical disciplines. For example, by using Hückel theory it is rather simple to draw the connection between conjugated π-systems in organic chemistry and semiconductors in solid-state chemistry.

3) A basic problem with textbooks for undergraduate teaching is that they react rather slowly on new developments. Many textbooks on conceptual chemistry have a large overhead with regard to topics, which are no longer suited for modern teaching. Therefore, the course includes new important developments from the current literature that will lead to a rewriting of textbooks in the future. Examples are Shaiks and Hiberty's revolutionary ideas on aromaticity or the modern understanding of the chemical bond in terms of the properties of the electron density distribution.

Specific Learning Objectives:

1) At the end of the course, the student will understand that the properties of atoms and molecules are a direct consequence of their electronic structure.

2) Furthermore, the student will understand the electronegativity concept and will be able to use it for solving chemical problems in connection with bonding, stability, and reactivity.

3) Orbital Theory: The student will be able to construct the orbitals of a simple molecule and to derive from their form an insight into the structure and stability of the molecule.

4) Chemical Bond: The student will understand that this is just a concept rather than a directly observable entity. Advantages, disadvantages, and complications of this concept will be understood by the end of the course.

5) Structure Diagrams: Given the frontier orbitals of a AH_n or AH_nBH_m molecule the student will be able to predict its preferred structure.

6) Stability: The student will understand the relationship between molecular structure and molecular stability.

7) Jahn-Teller effects: The student will understand the nature of a highly symmetrically degenerate molecular state and its tendency to deform.

8) Electron delocalization: The student will understand the quantum mechanical nature of electron delocalization and how this leads to unusual chemical behavior.

9) Aromaticity: The student will understand the concept of aromaticity and its implications for organic, inorganic, and transition metal chemistry

10) Potential Energy Surface: The student will understand the concept of the potential energy surface and will be able to derive from there the reactive behavior of well-defined compounds.

11) Molecular symmetry: The student will understand the importance of molecular symmetry for the understanding of the properties of molecules.
12) Orbital and spin symmetry conservation principles: The student will be able to understand these principles as the basis for reactivity predictions.
13) Woodward Hoffmann rules and Evans-Dewar Zimmermann rules: The student will be able to use these rules to correctly predict the outcome of chemical reactions.
14) Hypervalent molecules: The student will be able to explain the bonding in hypervalent molecules and to predict their properties.
15) Transition metal structures: The student will be able to derive their electronic structure and to predict the properties of simple transition metal complexes by investigating the corresponding orbital diagram.
17) Electron counting rules: Using these rules, the student will be able to understand stability and reactivity of metallocenes and other typical transition metal complexes.
18) Isolobal analogy: Using the concept of isolobal groups, the student will be able to relate chemical features of transition metal chemistry to those of organic or inorganic chemistry.
19) Cluster compounds: The student will understand structure and stability of simple cluster compounds.
20) Excited states: A basic understanding of excited states and their properties will be obtained by the student.

General Education Learning outcomes:
Science and Technology
1) Students will be able of demonstrating basic facility with the methods and approaches of scientific inquiry and problem solving.
2) Students will be able of explaining how the concepts and findings of science in general, or of particular sciences, shape our world.

5. Course Outline:
The course covers in 17 chapters major concepts and models used in chemistry. Some keywords describing the chapters are given in parentheses.

1. Atomic and Molecular orbitals (basic facts from MO theory; representation of orbitals; energy diagrams; LCAO-MO approach)
2. Theory of the Chemical Bond (MO description of the bond; electron density description; quantum mechanical description; orbital overlap; bonding in diatomic molecules; electronegativity and bond polarity; PE spectroscopy)
3. Structure of Molecules (Principle of maximum overlap; hybridization; bond orbitals; VSEPR model; the direct valence model)
4. Mulliken-Walsh MO model (Walsh diagrams for AH_n (n = 2,3,4), HAB, H_2AB, H_nAAH_n (n=1,2,3) molecules)
5. PMO Model (basic formulas; 1,2,3,4-electron cases; first and second order Jahn-Teller effects)
6. Hückel MO model σ–π-separation (Hückel theory; aromaticity concept)
7. Classical Mechanics applied to chemistry (concepts of strain; molecular mechanics; heats of formation from group increments; molecular modeling)
8. Interactions between orbitals (hyperconjugation; anomeric effect; through-space and through-bond interactions; homoconjugation and homoaromaticity; spiroconjugation)

9. Conformation and configuration of molecules (Rotational potential of single rotor molecules; Fourier expansion of potential; electronic effects that determine rotational potential; steric repulsion and steric attraction; cis-effect)
10. Theory of Pericyclic reactions (The Woodward-Hoffmann rules: orbital symmetry analysis; cycloadditions; electrocylic reactions; sigmatropic rearrangements; cheletropic reactions)
11. Evans-Dewar-Zimmermann concept (Evans principle; Hückel and Möbius systems; Dewar-Zimmermann rules)
12. Hypervalent Molecules (orbitals and bonding; pseudorotation in AH_5)
13. Transition metal chemistry: Basic Facts and Important Terms (nomenclature; role of transition metal complexes in chemical industry; generalized MO diagrams and electron counting rules)
14. ML_6, ML_5 and ML_4 Complexes (octahedral ML_6 complexes; high spin and low spin complexes; square planar and tetrahedral ML_4 complexes; square pyramidal and trigonal bipyramidal ML_5 complexes; ML_n complexes in Biochemistry)
15. ML_n Fragments (Lego-principle of MO diagrams; ML_2, ML_3, ML_4, and ML_5 fragments and their orbitals)
16. Metallocenes and Sandwich Complexes ($CpML_3$ complexes; CpM fragment orbitals; sandwich complexes)
17. The isolobal Analogy (isolobal fragments; cluster orbitals; capped annulenes; Wade rules).

Teaching Methodology: Lectures combined with exercises, assigned readings, class discussions, and student presentations. A computer lab complementing lectures and exercises will provide training possibilities.

6. Student Responsibilities:
Since the course content is not summarized in any of the available books, it is mandatory for each student to attend lecture hours and exercises. Although attendance will not necessarily lead to a better grade, attendance is a prerequisite for being accepted for the student presentations, the quizzes, and the final exam. Any problems, which might come up in this connection should be discussed without delay with the course instructor.

7. Final Examination: Day and time TBD.

8. Grading Procedures:
Grades are based on the degree of learning and competence demonstrated in the quizzes, the exercises, student presentations, and the final exam. Final grades will be calculated according to the following scheme:

Quizzes	30 %
Student presentation	10%
Exercises	20%
Final exam	40%

Grading Table	A	100 – 90 %

B	89 – 80 %
C	79 – 70 %
D	69 - 60 %
F	59% and below

Any problem with the final grading must be discussed with the course instructor within 8 days from the day of the return of the final exam

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 and worked out to accommodate best to the student needs.