Syllabus - CHE 417 / CHE 5417
Theoretical Chemistry

Spring Semester 3 semester hours credit

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Instructional Materials:
The required texts are ***Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics*** by Errol Lewars and ***Quantum Mechanics Demystified*** by David McMahon. In addition to these texts you will need a scientific calculator. Many of the class notes will be distributed.

Prerequisites: CHE 318. In addition to this specific prerequisite, students enrolled in CHE 5417 must have previously completed at least eighteen hours of chemistry.

Disclaimer: Although I expect to conduct the course according to the following, I reserve the right to make modifications if circumstances dictate.

Course Description: A study of theoretical chemistry, chemical physics, theoretical molecular spectroscopy, and solid-state chemistry with emphasis on fundamentals of quantum mechanics, vibrational and rotational spectroscopy, crystallography, and molecular electronic spectra.

Rationale: The expanding role of quantum chemistry makes it highly desirable for students in all areas of chemistry to understand modern methods of electronic structure calculation. In particular, theoretical chemistry is essential for a thorough understanding of bonding theories and spectroscopy. As in all physical chemistry courses at Mississippi College, development of problem solving and critical thinking skills are stressed.

Academic integrity: Mississippi College students are expected to be honest. Please refer to the *Mississippi College Undergraduate Bulletin* or to the *Mississippi College Graduate Catalog* for a discussion of plagiarism and cheating. Also refer to the *Mississippi College Tomahawk* or to University Policy 2.19.

Attendance: Your attendance at all class meetings is expected. Please refer to the *Mississippi College Undergraduate Bulletin* or to the *Mississippi College Graduate Catalog* for a discussion of the university's attendance policy. If a regular class meeting is missed, it is the student's responsibility to obtain any assignments or instructions that were given by the instructor. Missing a class is **not** an excuse for not preparing for the next class meeting or not having an assignment ready on time.

Methods of Instruction: Class will consist primarily of lectures and working problems. Occasionally, students enrolled in CHE 5417 will be required to present oral reports to the rest of the class.

Required Practices: You are expected to read the appropriate sections of your text and work any problems assigned before coming to class. Periodically throughout the semester special problem sets will be distributed which must be completed for a grade. Some of these problem sets will involve computational problems which will require the use of computational chemistry software located in the chemistry computer labs. The grades from all of the problem sets will be added to quiz grades as discussed below. Students enrolled in CHE 5417 will have additional computational problems assigned. In addition, CHE 5417 students will be required to prepare reports on special topics periodically throughout the semester and present these reports orally to the rest of the class. Finally, as previously mentioned, all students will need a good scientific calculator and be fairly proficient with it.

Grading: Two tests will be given during the semester, each with a value of 100 points. Unannounced pop tests are given periodically, the total number of pop test points and points from homework assignments will be approximately 100. Pop tests that are missed are not made up. The final exam is comprehensive and is worth 150 to 200 points. Your overall grade is determined by dividing your grand total by the total possible points. Occasionally there are opportunities for extra credit points by attending a special seminar or a visiting lecture.

CHE 417: Final letter grades are determined on a 10-point scale. Please refer to the *Mississippi College Undergraduate Bulletin* for a discussion of the university's grading system and how quality points are assigned.
CHE 5417: In addition to the above, approximately 100 points may be earned from the periodic reports and oral presentations mentioned above. Final letter grades are determined on the following scale:

90 -100 % = A	68 - 74 = C+	45 - 54 = D
84 - 89 % = B+	55 - 67 = C	below 45 = F
75 - 83 % = B		

Please refer to the *Mississippi College Graduate Catalog* for a discussion of the university's graduate grading system and how grade points are assigned.

Course Overview: The course covers material presented in chapters 1-12 of the McMahon text and chapters 1-8 of the Lewars text. The McMahon text presents an introduction to quantum mechanics. Three of the twelve chapters are devoted to the mathematical structure of quantum mechanics and another chapter to its foundations. This text will be covered quickly because much of its information will have been covered to some degree in Chemical Energetics (CHE 318). The Lewars text will be the primary text for the majority of the semester. It begins with a discussion of what computational chemistry is and what questions it can address. Chapter 2 presents the concept of the potential energy surface, and Chapter 3 discusses molecular mechanics. Chapter 4 introduces quantum mechanics into computational chemistry, and the next three chapters present the three major divisions of quantum mechanical calculations - ab initio methods (Chapter 5), semiempirical methods (Chapter 6), and density functional calculations (Chapter 7). The final chapter presents some model computational problems from the chemical literature and briefly discusses different computational chemistry software packages.

Learning Objectives: (This is not an exhaustive list.)

1) Learn to use differential and integral calculus in chemical and physical problems.
2) Learn how to compute the nth root of a complex number by using De Moivre's theorem.
3) Learn how to compute commutators.
4) Learn how to compute probabilities beyond the classical turning points for the quantum-mechanical one-dimensional harmonic oscillator.
5) Learn how to use ladder operators to generate eigenfunctions for another operator.
6) Learn the axioms of modern quantum theory.
7) Learn how to solve the problem of a particle in a three-dimensional infinite square-well potential.
8) Learn what the term *degenerate* means in quantum mechanics.
9) Learn what the virial theorem says and what it means.
10) Learn what the Hellmann-Feynman theorem says and what it means.
11) Learn how to generate the Hermite polynomials.
12) Learn how to solve the problems of a particle on a ring and a particle on the surface of a sphere.
13) Learn how the molecular Hamiltonian may be divided between the electronic and the nuclear Hamiltonians.
14) Learn how to calculate the energy levels in conjugated pi systems using simple Hückel theory.
15) Learn what SCF theory means and how it works.
16) Learn how to apply SCF theory to a problem of chemical interest via a computational chemistry software package.
17) Learn how molecular mechanics differ from quantum mechanical applications.
18) Learn how semiempirical methods, *ab initio* methods, and density functional theory methods differ.
19) Learn Koopman's Theorem.
20) Learn what electron correlation is, why it is important, and different ways to calculate it.
21) Learn why density functional theory is not an *ab initio* method, but may be as accurate or more accurate than some of them.
22) Learn what molecular properties may be computed with computational chemistry packages in addition to the energy.