Syllabus - **CHE 318 - Chemical Energetics**

Spring Semester — 4 semester hours credit
Class: MCC Building, Legg Conference Room — MWF 11:00 - 11:50 AM
Laboratory: Hederman Science Building, Room 405 — M 1:30 - 4:30 PM

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Instructional Materials:
The required text is *Physical Chemistry, 2nd edition* by Thomas Engel and Philip Reid. In addition to this text you will need a scientific calculator. General procedures for individual laboratory experiments will be distributed as well as many of the class notes.

Prerequisites: Differential and integral calculus, general physics, and CHE 317.

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

Course description: An introduction to the theoretical and fundamental aspects of quantum mechanics, molecular bonding and structure, and atomic and molecular spectroscopy.

Rationale: Physics is the fundamental science, while chemistry is the central science. Thus, this course in physical chemistry, as well as Chemical Dynamics, are studies of the fundamentals of the central science. It not only presents the underpinnings for much of the chemistry which a student has already encountered, it provides a foundation in physical chemistry for all future chemical study. Specifically, the fundamentals of quantum mechanics covered in Chemical Energetics provide a basis for bonding theories studied in Advanced Inorganic Chemistry and for additional studies of spectroscopy covered in Instrumental Analysis. In Chemical Energetics, as in Chemical Dynamics, development of problem solving and critical thinking skills are stressed.

Grading: Three tests will be given during the semester, each with a value of 100 points. These tests will most likely be given after the general theory of angular momentum is covered, after the study of molecular symmetry and group theory, and near the end of the semester. Unannounced pop tests are given periodically, the total number of pop test points and points from homework assignments will be approximately 50. Pop tests that are missed are not made up. The final exam is comprehensive and is worth 200 points. Laboratory participation, laboratory computer assignments, and lab reports together total 125 points. The course grade is determined by dividing your grand total by the total possible points. Final letter grades are determined on an 11-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.

Attendance: Your attendance at all class meetings is expected. Please refer to the *Mississippi College Undergraduate Bulletin* for a discussion of the university's attendance policy. Absences are recorded on the grade report that is mailed at the end of the semester. 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. **Do not miss a scheduled test!** In the event of an extreme emergency and an excused absence, a make-up test will be given. The test must be made up prior to the graded tests being returned to the class. Make-up tests are usually different from the regular test and may be more difficult. If the student cannot return to class until after the tests have been returned, the grade on the final exam may be substituted for the missing grade.

Methods of Instruction: Class will consist primarily of lectures and working problems. Occasionally we will go to the Chemistry Computer Lab to work problems with a spreadsheet or with Mathcad, a technical computation and visualization program developed and marketed by Mathsoft, Inc. in Cambridge, MA.

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. These grades will be added to quiz grades as discussed above. Also, as previously mentioned, you will need a good scientific calculator and be fairly proficient with it.

Course and Lab Overview: The course covers material presented in chapters 12-28 of the textbook. The laboratory provides the opportunity to measure physical and chemical constants related to the theory studied in class. In addition to demonstrating established principles and reinforcing and expanding one's understanding of the basic concepts, the lab should help to develop research aptitudes by providing experience with the types of experiments and instrumentation that can yield new results in a given field. Statistics will be emphasized in determining how precisely a given physical or chemical constant was measured. In short, the aim is to train not lab techs, but research scientists.

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

Brief Course Outline:

I. Introduction to Quantum Mechanics

- A. Beginnings
  1. Blackbody radiation and Max Plank
  2. Photoelectric effect and Albert Einstein
  3. Neils Bohr and his theory of the atom
  4. Wave-particle duality
  5. Modern quantum theory discovered - Schrödinger, Heisenberg, and Dirac
- B. Operator Algebra
  1. Eigenfunctions and eigenvalues

2. Commutators
3. Ladder operators
4. Heisenberg Uncertainty Principle
5. Schrödinger's Equation

C. Model Systems
1. Particle in an infinite-square-well potential
2. One-dimensional harmonic oscillator
3. Rigid Rotor

D. General Theory of Angular Momentum
1. Orbital angular momentum
2. Spin angular momentum

II. Atomic Structure

A. Solutions for the Hydrogen Atom
1. Atomic orbitals
2. Spin functions

B. Polyelectron atoms
1. Atomic orbital approximation
2. Atomic Term Symbols and Hund's Rules

C. Atomic Spectroscopy

III. Approximation Methods

A. Variational Theory

B. Perturbation Theory

IV. Molecular Structure

A. Molecular Symmetry and Group Theory

B. Born-Oppenheimer Approximation

C. Nuclear wavefunctions
1. Potential energy surfaces
2. Infrared spectroscopy
3. Raman spectroscopy

D. Electronic wavefunctions
1. LCAO-MO approximation
2. Diatomics
   a. Bonding and antibonding molecular orbitals
   b. Occupied and virtual molecular orbitals
   c. Bond order
3. Hückel theory

V. Lasers

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

1) Learn to us differential and integral calculus in chemical and physical problems.
2) Learn how quantum mechanics arose from problems and unanswered questions in classical mechanics.
3) Learn how Max Planck solved the problem of blackbody radiation.
4) Learn how Albert Einstein solved the problem of the photoelectric effect.
5) Learn Neils Bohr's model of the atom.
6) Learn the equation of Louis de Broglie and how to use it.
7) Learn the men who discovered modern quantum theory.
8) Learn what an eigenfunction/eigenvalue equation is.
9) Learn how to compute a commutator.
10) Learn how ladder operators can generate eigenfunctions for another operator.

11) Learn the postulates of modern quantum theory.
12) Learn how to solve the problem of a particle in an infinite square-well potential.
13) Learn how to apply the solution of the particle in an infinite square-well potential to model electron spectroscopy.
14) Learn what the Bohr Correspondence Principle is.
15) Learn what the term *degenerate* means in quantum mechanics.
16) Learn what the Heisenberg Uncertainty Principle says and what it means.
17) Learn how to solve the problem of the quantum-mechanical one-dimensional harmonic oscillator.
18) Learn what the Hermite polynomials are.
19) Learn how to apply the solution of the quantum-mechanical one-dimensional harmonic oscillator to model infrared spectroscopy.
20) Learn how to solve the problem of a particle on the surface of a sphere.
21) Learn what the spherical harmonics are.
22) Learn how orbital angular momentum and spin angular momentum differ.
23) Learn how to couple angular momentum vectors.
24) Learn what hyperfine splitting is and how atomic clocks work.
25) Learn how to apply the solution of the particle on the surface if a sphere to rotational spectroscopy.
26) Learn how temperature affects rotational spectroscopy via a Boltzmann distribution.
27) Learn which regions of the electromagnetic spectrum are associated with the different types of spectroscopy.
28) Learn the basic properties of the hydrogenic orbitals.
29) Learn how to determine atomic term symbols associated with electron configurations.
30) Learn what symmetry elements are used to describe the symmetry in molecules.
31) Learn how to classify molecules by their symmetry point group.
32) Learn what a matrix representation of a group is.
33) Learn how to determine how many irreducible representations a given group has.
34) Learn to reduce reducible representations into irreducible representations.
35) Learn how to take direct products of matrix representations.
36) Learn how symmetry is relevant to problems in quantum mechanics and spectroscopy.
37) Learn what the Born-Oppenheimer approximation is.
38) Learn how the molecular Hamiltonian may be divided between the electronic and the nuclear Hamiltonians.
39) Learn how to calculate the energy levels in conjugated pi systems using simple Hückel theory.
40) Learn what SCF theory means and how it works.