PHYSICAL CHEMISTRY I:  
Quantum Mechanics and an Introduction to Statistical Thermodynamics

INSTRUCTOR: 
Section A: Prof. David Wu  
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TEXTBOOK: 
Physical Chemistry: A Molecular Approach  
by McQuarrie and Simon

COURSE TIMES: 
MWF 1:00-1:50  
Section A: Berthoud 201  
Section B: Brown 201

LAB COURSE: 
starts the second full week  
Wet Labs will be held in Coolbaugh Hall 320  
Dry Labs will be held in the Green Center and other locations

PREREQUISITES: 
CHGN 124, DCGN 209, MACS 315

EXAMS: 
Two take-home exams approximately 1/3 and 2/3 into semester.

HOMEWORK: 
Solutions are available, but credit will not be given for simply copying the answers. To get full credit, you need to explain what is the significance of the question or answer.

GRADING: 
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<th>Component</th>
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<tbody>
<tr>
<td>Participation</td>
<td>25%</td>
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<tr>
<td>Homework</td>
<td>10%</td>
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<tr>
<td>Exam 1</td>
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<td>Exam 2</td>
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<td>Lab</td>
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* All labs must be completed to receive a grade in CHGN 351.
COURSE PHILOSOPHY

Physical chemistry is a demanding subject due both to its exceptional breadth and to its rigor. It is, however, these same two qualities which makes it so useful in scientific or engineering endeavors. The building of knowledge is both horizontal (varied principles) and vertical (principles building on each other).

Quantum mechanics represents a radical and classically non-intuitive (counter to “common sense”) way of thinking about physical phenomena. To help develop intuition, a simple exercise or question, meant to stimulate reflection, will regularly be given in class and discussed briefly in the following class. Before discussion, we may occasionally ask for written answers (a paragraph or so) to help us make sure the ideas are getting across, and will count a small amount towards grading. There will also be approximately weekly graded homework assignments to allow you to sink your teeth into more involved questions, and to let you develop some of the basic problem-solving skills.

PARTICIPATION

You will be expected to take responsibility for your learning and progress in this course. Part of this process is your active participation, both in the classroom and outside. In the classroom, you will be expected to actively engage in discussions and question, and you will occasionally be expected to prepare material for the entire class. Outside of class, you are required to keep a diary of your learning progress (questions that occur to you, etc.), as well as participate in the on-line class bulletin board.

COURSE OUTLINE

The first three-quarters of the course will be devoted to quantum chemistry, while the last quarter (following spring break) will be an introduction to the fundamentals of statistical thermodynamics. The first part will follow McQuarrie’s Physical Chemistry fairly closely, whereas the second part may also draw from the references listed below as needed.

Here is a rough schedule, which can be altered to suit the needs and interests of the class:

I. Introduction to Physical Chemistry (1 week)
   A. Structure & Properties, Heat Capacity and Potentials
   B. Atoms and Molecules: Energies, Sizes, Speeds…

II. Quantum chemistry (9 Weeks).
   A. Historical aspects, atomic spectra, the Bohr model, wave-particle duality
   B. Classical wave motion and normal modes
   C. The Schrödinger Equation and the Particle In a Box
   D. Postulates of quantum mechanics and application to simple systems.

III. Statistical Thermodynamics (4 Weeks)
   A. Review of classical thermodynamics and fundamental postulates
   B. Derivation of Boltzmann’s entropy
   C. Ensemble theory and the canonical ensemble
   D. Heat Capacity Revisited
COURSE OBJECTIVES

1. To provide a deeper understanding of the physical chemistry principles introduced in introductory chemistry courses and distributed core thermodynamics
2. To teach students the fundamental concepts and methods of quantum mechanics to prepare for the application of these principles to the study of atoms and molecules, including chemical bonding and spectroscopy. Modern computational methods as applied to physical chemical problems will be part of this process
3. To develop in students an understanding of statistical thermodynamics including fundamental postulates, Boltzmann’s entropy, ensemble theory, canonical ensemble, and phase transitions
4. To provide students a molecular-based understanding for learning further advanced topics and domains of physical chemistry to be covered in CHGN 353, such as chemical kinetics, catalysis, electrochemistry, surface and macromolecular chemistry
5. To provide the knowledge and intuition of molecular scale processes that allow rationalization of how molecular scale parameters can affect macroscopic properties

Quantum Chemistry

1. To build intuition for the radical concepts introduced by the quantum theory
2. To acquire proficiency in attacking and solving quantum chemical problems--skills needed for future work in molecular level science and engineering
3. To have an appreciation for the historical context, as well as the startling philosophical consequences of the quantum theory
4. To enable critical and intelligent use of quantum computational software packages, which are becoming a standard tool in research and industry

Statistical Thermodynamics

1. To be introduced to the fundamental principles of statistical mechanics, and the relationship to macroscopic observations
2. To develop a sense of the scope of application of statistical thermodynamic principles--when would these ideas be useful in practical situations
3. To gain a rudimentary facility with computational methods of statistical mechanics
OTHER REFERENCES

Quantum Chemistry

1. Quantum Chemistry, Donald A. McQuarrie
2. Quantum Chemistry, 4th Ed., Ira N. Levine
3. An Introduction to Quantum Physics, A.P. French and E.F. Taylor
4. Atoms and Molecules, Martin Karplus and Richard N. Porter
5. What is Quantum Mechanics?: A Physics Adventure, by Transnational College of LEX

Statistical Thermodynamics

6. Fundamentals of Statistical and Thermal Physics, Frederick Reif
7. Statistical Mechanics, Donald. A. McQuarrie
8. Thermodynamics and an Introduction to Thermostatistics, 2nd Ed., Herbert B. Callen
9. Introduction to Modern Statistical Mechanics, David Chandler

LABORATORY

The accompanying laboratory period will consist of matched “wet” and “dry” exercises in alternating weeks, loosely following the progress of the lecture material. These laboratory exercises will develop concepts such as the application of simple particle-in-a-box concepts to spectra of dye molecules; wave nature of matter and the mathematical description in terms of basis sets; intermolecular potentials and structure as reflected in electronic, vibrational and rotational and spectroscopy; application of computational chemistry software (such as SPARTAN) to chemical problems such as kinetics and transition state determination; thermodynamic measurements and statistical mechanical calculations based on microscopic structure.