Chem 332

Physical Chemistry II – Quantum Mechanics

Spring 2016

Course Information

Instructor: Dr. David Y. Lee

Office: 104A Fulmer Hall **Lab:** N117 Fulmer

Phone: 5-9773 **e-Mail:** d.y.lee@wsu.edu

Office Hours: 3 pm Monday and 3 pm Friday; or by appointment.

Prerequisite: MATH 273 with a C or better; MATH 220 with a C or better; PHYSICS 202 with a C or better

Textbook:
Physical Chemistry — A Molecular Approach by *D. A. McQuarrie* and *J. D. Simon*
(Supplementary) The Chemistry Maths Book by *E. Steiner*

Evaluation:
Homework: 35%
Two In-Class Exams: 40%
Cumulative Final: 25%

Grading Scale:
85–100% **A**
80–84.9% **A– / B+**
70–79.9% **B**
65–69.9% **B– / C+**
56–64.9% **C / C–**
50–55.9% **D**
≤50% **F**

Homework: The key to learning physical chemistry is working and thinking about problems. Many students find that they learn and retain more if they discuss challenging problems with one another. You are therefore encouraged to discuss (not to share solutions of) the homework problems with other members of the class. However, every student is responsible for his/her own writeup. The ground rules are:

> You may not copy and/or edit another students work and submit it as your own, either in full or in part. You may not jointly edit or compose solutions with another student. ***Use of solution manuals for homework sets is inappropriate and is considered cheating***. Homework sets will be due in lecture. Late homework sets will not be accepted.

Exams: There will be two equally weighted prelims. No make-up prelims will be given. If an exam is missed because of illness or a pre-approved absence, an estimated grade will be assigned on the basis of the other examinations. ***The final exam will be cumulative***.

WSU Academic Integrity Statement

"As an institution of higher education, Washington State University is committed to principles of truth and academic honesty. All members of the University community share the responsibility for maintaining and supporting these principles. When a student enrolls in Washington State University, the student assumes an obligation to pursue academic endeavors in a manner consistent with the standards of academic integrity adopted by the University. To maintain the academic integrity of the community, the University cannot tolerate acts of academic dishonesty including any forms of cheating, plagiarism, or fabrication. Washington State University reserves the right and the power to discipline or to exclude students who engage in academic dishonesty."

Students found responsible for academic integrity violations may receive an **F** on the particular assignment or exam, as well as an **F** for the course. Repeated and/or serious offenses may result in referral to the conduct board and **expulsion from WSU**. For graduate students, academic integrity violations may also result in the loss of teaching and/or research assistantships.

Students with Disabilities

Reasonable accommodations are available for students with a documented disability. If you have a disability and need accommodations to fully participate in this class, please either visit or call the Access Center (Washington Building 217; 509-335-3417) to schedule an appointment with an Access Advisor. All accommodations MUST be approved through the Access Center.

Course Outline:

1. **Prelude: Fast Introduction/Review of Matrix Algebra**
   - The 2D Rotation Matrix
   - Inverse and Orthogonal Transformation
   - Eigenvalues and Eigenvectors; Matrix Diagonalization
   - Hermitian Matrices
2. **Classical Mechanics**
   - $\boldsymbol{F} = m\ \boldsymbol{a}$
   - Fourier Analysis
   - Lagrangian Formulation
   - Hamiltonian Formulation
3. **The Need for Quantum Mechanics**
   - Blackbody Radiation
   - Line Spectra
   - Bohr's Atomic Model
   - Photoelectric Effect
4. **Wave (State) Equations for Matter**
   - De Broglie Waves
   - The Uncertainty Principle
   - The Schrödinger Equation
   - The Hydrogen Atom
   - Pauli Exclusion Principle and the Spin Quantum Number
   - Shell & Subshells; Removal of Degeneracy
5. **Hilbert Space**
   - The Correspondence Principle and the Copenhagen Interpretation
   - Average Values Superposition
   - Hermitian Operators and Orthonormal Eigenfunctions
6. **Boundary Conditions & Quantization of Energy**
   - Curvature, Sign and Acceptability of the Wavefunctions
   - Penetration into Non-Classical Regions
   - Particle in a Box
   - Harmonic Oscillator

7. **Angular Momentum in QM**
    - Angular Momentum in CM
    - Angular Momentum Operators, Matrix Elements and Eigenfunctions
    - Addition of Angular Momentum and Clebsch-Gordan Series
    - Spin
8. **Molecular Spectroscopy**
    - Vibrational
    - Rotational
9. **Multi-Electron Problems**
    - He Atom
    - Antisymmetry of the Wavefunctions
    - Slater Determinants
    - Term Symbols
    - Atomic Spectroscopy
10. **Approximation Methods**
    - The Variation Principle
    - Perturbation Theory
11. **Fundamental Theory of Chemical Bonding**
    - The Born–Oppenheimer Approximation
    - H_2^+
    - Molecular Orbitals
12. **Molecular Structure of Polyatomic Molecules**
    - Hybridization
    - Molecular Orbital Theory
    - Hückel Method