Instructor: Prof. David Y. Lee
Office: 118 Fulmer
Phone: 5-9773
Office Hours: Free to stop-by when my door is open 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; *CHEM 330

Textbook:
Physical Chemistry — A Molecular Approach by D. A. McQuarrie and J. D. Simon

Evaluation:
Homework and Class Exercises: 20%
One Mid-Term Computational Project (based on skills learned in Chem330): 15%
Three In-Class Exams (ALL Cumulative):
Exam #1: 20%
Exam #2: 20%
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

General: It has been shown that in a simple lecture setting students only learn about 10% of what they are told. If the students stay active in participating in class, that can be pushed to about 50% but the amount of material covered decreases considerably. Moreover, in the time we have for lecture, I will only be able to talk about 25 to 30% of what is in the text. Bottom line is that I am not going to be able to pour knowledge into your head - at this stage of your college career you should have possessed the skills of learning science on your own in a comprehensive fashion - and hopefully with my help this learning experience will be a lot easier. So, read the textbook as the course progresses and be prepared to ask questions. Do each problem until you can do it with the book closed. Stay awake and participate in the classroom exercises. And remember, you are not learning the material for my exams, you are learning it for your own benefit as a scientist or engineer.
**Homework and Class Exercises:** 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 will be assigned into specific study groups and have many chances to lead the entire class in solving problems.

**Mid-Term Projects:** You will need either Mathematica or MATLAB with skills gained in Chem330. You may **NOT** copy and/or edit another student's work and submit it as your own, either in full or in part. You may **NOT** jointly edit or compose solutions with another student.

**Exams:** There will be three exams, and no make-up exams 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. *ALL the exams will be cumulative.*

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**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.

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**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 (tentative):

1. **Prerequisite: Basic Matrix Algebra** (already reviewed in Chem330)
   - The 2D Rotation Matrix
   - Inverse and Orthogonal Transformation
   - Eigenvalues and Eigenvectors; Matrix Diagonalization
   - Hermitian Matrices

2. **Why We Need Quantum Mechanics**
   - M&S Ch. 1-1 to 1-7
   - Blackbody Radiation
   - Photoelectric Effect
   - The Hydrogen Atomic Spectrum
   - de Broglie Waves

3. **Classical Mechanics**
   - $F = ma$
   - Fourier Analysis
   - Lagrangian Formulation
   - Hamiltonian Formulation

4. **Wave (State) Equations for Matter**
   - *The Schrödinger Equation*
   - The Hydrogen Atom
   - The Uncertainty Principle
   - 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
    - $\text{H}_2^+$
    - Molecular Orbitals

12. **Molecular Structure of Polyatomic Molecules**
    - Hybridization
    - Molecular Orbital Theory
    - Hückel Method