

B.S. Junior Year – Fall Semester Lecture

CEM 483 Quantum Chemistry

Description: Postulates of quantum mechanics and their application to model systems, atoms and molecules. Introduction to molecular spectroscopy.

Credit: 3 hours (3 hours lecture and 1 hour recitation per week)

Prerequisite: (CEM 142 or CEM 152 or CEM 182H or LB 172) and (MTH 235 or MTH 255H) and (PHY 184 or PHY 284H); Recommended background: One year of general chemistry, calculus through differential equations and general physics. SA: CEM 362, 461. Not open to students with credit in CEM 384.

Lecture Topics:

1. Pivotal Experiments and Ideas Leading to the Development of Quantum Mechanics
2. Classical Wave Equation (optional)
3. Time-Independent Schrödinger Equation, Operators, and Eigenvalue Equations
4. Postulates of Quantum Mechanics (Mathematical Properties of Wave Functions; Quantum Mechanical Operators and Commutators; Expectation Values; Time-Dependent Schrödinger Equation)
5. Model Problems (Particle in a Box; Harmonic Oscillator; Rigid Rotator, Angular Momentum, and Spherical Coordinates)
6. Hydrogen Atom
7. Approximation Methods (Perturbation Theory; Variational Method and Secular Determinants)
8. Multi-electron Atoms (Electron Spin and Spin Angular Momentum Operators; Pauli Exclusion Principle; Slater Determinants; Atomic Term Symbols; Hund's Rules, and Spin-Orbit Coupling)
9. Bonding in Diatomic Molecules (Born-Oppenheimer Approximation; Linear Combination of Atomic Orbitals and Molecular Orbital Designations; Overlap, Coulomb, and Exchange Integrals; Molecular Term Symbols)
10. Bonding in Polyatomic Molecules (Molecular Orbital and Valence Bond Theories; Hückel MO Theory)
11. Molecular Spectroscopy: Transition Energies and Selection Rules (Rotational, Vibrational, and Electronic)
12. Computation Chemistry, if time permits
13. Mathematical tools, introduced throughout the semester as needed

Notes:

The material on the topic list for CEM 483 is found in Chapters 1-13 of the textbook *Physical Chemistry: A Molecular Approach* by D. A. McQuarrie and J. D. Simon.