

JNC307 (Jan) 3:0

Quantum Chemistry and Chemical Bonding

- Basics: Energy quantization, wave particle duality, observation and probability, wave functions, Operators, Observables
- Quantization Principles; Schrodinger Equations; The Uncertainty Principle
- Exactly Solvable Problems: Free Particle, Particle in a box, Harmonic Oscillator, Hydrogen Atom
- Time independent Perturbation theory and Variational theory
- HatreeFock: A bird's eye view, spin orbit, slater determinants, unitary transformation
- Atomic and Molecular Structures: Pauli principle, classification of atomic spectra, Atomic Orbitals, Atomic Transitions and Spin
- Molecular Orbital Theory: H₂⁺ Molecule, Hydrogen Molecule from atomic orbitals – Bonding and non-bonding orbitals, Hybridization
- Electronic Configuration, term symbols, Exploiting Symmetry
- Molecular Orbitals of homo and hetero diatomic molecules, poly atomic molecules
- Results of HF – Orbital model of atom, nature of Chemical bond, Localization of Molecular orbitals, Molecular Geometry and VSEPR model, Shapes of polyatomic molecules, Conjugation and Resonance
- Molecules to Solids: Band Structure, Solid state quantum Chemistry – An Overview.

Reference books:

1. I. N. Levine, "Quantum Chemistry", 5th Edition, Allyn and Bacon
2. A. Szabo and N. S. Ostlund, "Modern Quantum Chemistry: Introduction to Advanced Electronic Structure", Courier Dover Publications.
3. Victor Gil, "Orbitals in Chemistry: A Modern Guide for Students", Cambridge University Press.
4. T. Engel and P. Reid, "Quantum Chemistry and Spectroscopy", Pearson Education Inc.
5. M. Kuno, "Introductory Nanoscience; Physical and Chemical Concepts", Garland Science.