

JCL 307 (Jan) (3-1-0)**Quantum Chemistry and Chemical Bonding*****Instructor: Ranjani Viswanatha***

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; Hatree Fock: A bird's eye view, spin orbit, slater determinants, unitary transformation

Study of electronic structure of metals and semiconductors from a quantum mechanical perspective, principle of scanning tunneling microscopy, Density of states in a particle in a box, Vibrational energy levels in an atom/ molecule.

Atomic and Molecular Structures: Pauli principle, classification of atomic spectra, Atomic Orbitals, Atomic Transitions and Spin; Molecular Orbital Theory: H_2^+ 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. Quantum Chemistry, I. N. Levine, 5th Edition, Allyn and Bacon
2. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure, A. Szabo and N. S. Ostlund, Courier Dover Publications.
3. Orbitals in Chemistry: A Modern Guide for Students, Victor Gil, Cambridge University Press.
4. Quantum Chemistry and Spectroscopy, T. Engel and P. Reid, Pearson Education Inc.
5. Introductory Nanoscience; Physical and Chemical Concepts, M. Kuno, Garland Science.