Paper-13C

Basics of Condensed Matter Physics

Group A: Basics of Condensed Matter Physics 1 **[36 Lectures]**

Lattice dynamics: Classical theory of lattice vibrations in 3-dimensions under harmonic approximation; Dispersion relation: acoustical and optical, transverse and longitudinal modes; Lattice vibrations in a monatomic simple cubic lattice; Lattice waves, vibrational modes and phonons; normal and soft modes; phonon-phonon interaction, Inelastic Neutron Scattering and lattice dynamical modeling; Neutron diffraction by lattice vibrations; Elastic constants of crystals, Mossbauer effect.

[16L]

Electronic transport properties: The Boltzmann transport equation and relaxation time; Electrical conductivity of metals, impurity scattering, ideal resistance at high and low temperatures, Umklapp-processes; Electronic properties in a magnetic field; Hall effect and magnetoresistance in two-band model; K-space analysis of electron motion in a uniform magnetic field; Thermoelectric effects; Energy levels and density of states in a magnetic field; Landau diamagnetism; Cyclotron resonance, de Haas-van Alphen effect; Quantum Hall effect.

[20L]

Reference Books:

1. N.W. Ashcroft and N.D. Mermin: Solid State Physics

2. M. Sachs: Solid State Theory

3. J.M. Ziman: Principles of the Theory of Solids

4. C. Kittel: Introduction to Solid State Physics

Group B: <u>Basics of Condensed Matter Physics 2</u> [36 Lectures]

Many-electron systems: Basic electron-ion Hamiltonian in a solid (Time dependent to Time independent); the adiabatic approximation; Self-consistent field approximation, single product and determinantal wave functions, Hartree and Hartree-Fock (H-F) theory: exchange interaction and exchange hole, Koopman's theorem; Occupation number representation: Many electron Hamiltonian in occupation number representation; H-F ground state energy; Inclusion of electron correlation via configuration interaction.

[18L]

Density Functional Theory: Fundamentals of DFT, comparison with conventional wave function approach, 1-body and 2-body Reduced Density Matrix, Electron Density as the basic variable, Thomas- Fermi model as precursor of modern DFT; Hohenberg-Kohn theorems; Functionals and functional derivatives; Euler-Lagrange formulation; Kohn-Sham equation; Concept of N- and v-presentability; Exchange-Correlation energy functionals; LDA, GGA and beyond; Practical implementations of DFT; Basis sets : Plane Wave and localized. Triumphs

and shortcomings of DFT for treating molecules, solids and nanomaterials.

[18L]

Reference Books:

1) Quantum Theory of Molecules and Solids, J.C. Slater, Vol IV (McGrawHill, New York, 1974).
2) Electronic structure and properties of solids, W.A. Harrison (Freeman, 1980).
3) "Theory of inhomogeneous electron gas", S Lundqvist and N.H. March, (Plenum, New York, 1983)
4) "Electronic Structure: Basic Theory and Practical Methods", Richard M. Martin (Cambridge University Press, 2004)