Department of Physics, University of Kashmir, Srinagar

Pre-PhD Course: Solid State Physics

Special Paper-III   Batch: 2023

UNIT 1

CRYSTAL and BAND STRUCTURE OF SOLIDS

Bravais Lattice, Point groups, Space groups, Miller Indices, Reciprocal Lattice, Bragg's Law in reciprocal space, X-ray diffraction, Scattering wave Amplitude, Brillouin Zones.

Nearly Free Electron Model, Bloch functions, Wave equation of electron in a periodic potential, Tight binding model.

UNIT 2

MANY-BODY SCHRODINGER EQUATIONS

Basic Equations for Interacting Electrons and Nuclei, Many-body Schrodinger equation, Independent electrons approximation, Exclusion principle, Mean-field approximation Hartree Method, Hartree-Fock equations, Self-Consistent field method.

UNIT 3

INTRODUCTION TO DENSITY FUNCTIONAL THEORY

Density functional theory: From wave function to electron density function, Thomas–Fermi model, Hohenberg-Kohn theorem, Kohn-Sham equations, the local density approximation, Exchange and correlation energies of the electron gas, Self-consistent calculations.

UNIT 4

DENSITY FUNCTIONAL THEORY OF CRYSTALS

Band structures, Kohn-Sham equations for a crystal, Kohn-Sham energies and wavefunctions, Calculation of band structures and Density of States using DFT, Plane wave methods, pseudopotentials. The band gap problem. Practical implementation of DFT using Quantum Espresso.

Recommended Books:

1. Electronic Structure: Basic Theory and Practical Methods

Richard Martin , Cambridge University Press

2. Materials Modelling Using Density Functional Theory

 Feliciano Giustino , Oxford Publishers.

3. Density Functional Theory: A Practical Introduction

David S. Sholl, Janice A. Steckel (John Wiley & Sons)

4. Electronic Structure Calculations for Solids and Molecules: Theory and Computational Methods,

Jorge Kohanoff , Cambridge University Press