

Approved: 2<sup>nd</sup> adhoc meeting.

**PH-505: Electronic Structure (3-0-0-3)**

1. Overview: Quantum theory and origin of electronic structure, electronic ground state, basic equations for interacting electron and nuclei, periodic solids and bands, uniform electron gas and simple metals. [7-8 Lectures]
2. Density functional theory : DFT foundations, Thomas Fermi Dirac approximations, Hohenberg-Kohn Theorems, intricacies of DFT, Kohn Sham variational equations, Time dependent DFT, local spin density approximation, GGA, LDA, solving Kohn-Sham equations [7-8 Lectures]
3. Important preliminaries on atoms: One electron Schrodinger equation, relativistic Dirac equation, atomic sphere approximations, pseudopotentials, orthogonalized plane waves, ultrasoft potentials, projected augmented waves [7-8 Lectures]
4. Determination of Electronic structure :Bloch Theorem, Nearly free electron model, ab initio pseudopotential method, crystal structure, supercells, clusters and molecules, tight binding methods, augmented functions: APW, MTO, linear methods, LAPW. [7-8 Lectures]
5. Predicting properties of matter from electronic structure- recent developments and computational resources in use. [7-8 Lectures]

**Text Book:**

Electronic Structure: Basic theory and practical methods, Cambridge University Press, 2004, R.M. Martin

**References:**

1. Electronic Structure: Basic theory and practical methods, Cambridge University Press, 2004, R.M. Martin
2. Ashcroft and Mermin, Solid State Physics, Holt, Rinehart and Winston, 1976
3. Kittel, Introduction to Solid State Physics, Wiley, 1986, pp. 228-239.
4. Omar, Elementary Solid State Physics, Addison{Wesley, 1975, pp. 189{210.
5. Ziman, Principles of the Theory of Solids, Cambridge, 1972, Chapter 3.
6. W. Hergert A. Ernst M. D'ane (Eds.) : Computational Materials Science: From Basic Principles to Material Properties
7. JMD Coey :Magnetic Materials