PH505 Electronic Structure

Credit: (3-0-0-3) Approval: Approved in 2nd Senate

Prerequisites: Quantum Mechanics

Students intended for: B.Tech

Elective or Core: Elective Semester: Odd/Even

Course objective: This course will provide a unified exposition of the basic theory and methods of electronic structure, together with instructive examples of practical computational methods and real-world applications. It will include the approach most widely used today – density functional theory – with emphasis upon understanding the ideas, practical approaches, and limitations. In addition, electronic structure is an interacting many-body problem that ranks among the most pervasive and important in physics.

Course content:

- 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]
- 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, soving Kohn-Sham equations [7-8 Lectures]
- 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]
- Determination of Electronic structure :Bloch Theorem, Nearly free electron model, ab initio pseudopotential method, crystal structure, supercelss, clusters and molecules, tight binding methods, augmented functions: APW, MTO, linear methods, LAPW. [7-8 Lectures]
- 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:

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

Ashcroft and Mermin, Solid State Physics, Holt, Rinehart and Winston, 1976

Kittel, Introduction to Solid State Physics, Wiley, 1986, pp. 228-239.

Omar, Elementary Solid State Physics, Addison{Wesley, 1975, pp. 189{210.

Ziman, Principles of the Theory of Solids, Cambridge, 1972, Chapter 3.

W. Hergert A. Ernst M. D¨ane (Eds.) : Computational Materials Science: From Basic Principles to Material Properties

JMD Coey :Magnetic Materials