PHY 621

Electronic Structure of Materials

Prereq. (For M.Sc. and Undergraduate students PHY 543, None for Ph.D. students)

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Knowledge of electronic structure is essential to understand electronic, magnetic, transport, optical and various other properties of materials. The course aims to give an overview of basic concepts involved and various approaches for calculating electronic structure. These approaches are based on the density functional theory. The course will be particularly useful for Ph.D. students who want to work in this area or want to understand their experimental results using electronic structure calculations. The students should have some knowledge of computer programming.

Course content:

One electron model, Born-Oppenheimer approximation, Hartree & Hartree-Fock approximation, density functional theory, local density approximation, beyond LDA. electrons in periodic solids, Bloch's theorem, nearly-free electron model, energy bands, Fermi surface, The tight-binding method, APW method, OPW method, pseudo-potential method, KKR method, LMTO method, the full-potential methods. applications to different types of solids; electron in disordered solids, mean-field theories, coherent potential approximation, KKR-CPA. Applications of KKR-CPA, tight-binding molecular dynamics, applications to clusters and solids, Car-Parinello methods and its applications to clusters and amorphous semiconductors, applications of electronic structure methods to materials design.

Reference Books:

1. Electronic Structure of Materials by R. Prasad
2. Electronic Structure by R. M Martin