

PHY 621 (II Semester 2009-10)

Electronic Structure of Materials

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

Instructor: R. Prasad

Office: FB 373, Phone: 7065, email: rprasad@iitk.ac.in

Classes: Monday, Thursday and Friday at 12 noon in FB482

Knowledge of electronic structure is essential to understand electronic, magnetic, transport 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. Project work will form an important component of the course. The students should have some knowledge of computer programming.

1. 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.

2. Reference Books:

1. Electronic Structure by R. M Martin
2. Electronic Structure by W. A. Harrison
3. Methods of Electronic Structure Calculations by M. Springborg

3. Attendance:

Attendance is compulsory in this course. One mark will be awarded for attending each class. You will not get this mark if you are late by more than 5 minutes. If you attended all the classes, 5 bonus marks will be awarded.

4. Evaluation will be based on following:

1. Project	100 Marks
3. End-Semester Exam	100 Marks
4. Attendance	1Mark /Class

5. Grading:

Grading will be relative. Students getting marks above the average may expect A or B; those getting below the class average may expect to get C and D grades. F will be awarded if the student scores less than 40% marks in aggregate.

6. Help:

If you need any kind of help, academic or personal nature, I encourage you to meet me as soon as possible. Do not wait till the exams are very near. Easiest way is simply to come to my office or you can send an email and get an appointment. However, please do not call my residence unless it is an emergency.