ELECTRONIC PROPERTIES OF THE MATERIALS: COMPUTATIONAL APPROACH

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PRE-REQUISITES : Basic physics (classical mechanics and electrodynamics), and mathematics.
INTENDED AUDIENCE : Introductory course
INDUSTRY SUPPORT : This is an introductory course for UG/PG students. However, companies dealing with semiconductor materials might be interested.

COURSE OUTLINE :

The course aims to explain the physics of electronic materials in detail, followed by a brief discussion on their applications. A student taking the course will learn about traditional metals, semiconductors, and ionic-conductors, as well as newly discovered low-dimensional materials. In addition to the theory part, students will also learn from simple in-silico experiments.

ABOUT INSTRUCTOR :

Prof. Somnath Bhowmick has been working in computational materials science related to the electronic and magnetic properties of the materials. He has eight years of teaching and research experience in the Department of Materials Science and Engineering, IIT Kanpur. He has taught several UG/PG compulsory and elective courses (as an instructor, as well as a tutor), like -- Electronic and Magnetic Properties of Materials (UG core course), Mathematics and Computational Methods (PG core course), Symmetry and Properties of Materials (UG/PG elective course), Introduction to Computer Simulations in Materials Science (UG/PG elective course), Quantum Physics (UG core course) and Partial Differential Equation (UG core course).

COURSE PLAN :

Week 1: Electronic materials in various applications,Introduction to the Drude model and failure of the classical theory,Introduction to Quantum Physics

Week 2: Basic introduction to Python programming ,Numerically solving Schrodinger equation, Numerov method and WKB approximation

Week 3: Free electron gas in ground state T=0 ,Free electron gas at finite temperature and electronic free energy calculation by numerical integration, Failure of free electron model (1 lecture), Introduction to the Bravais lattice and reciprocal lattice, Visualization of Bravais and reciprocal lattice (1 lecture

Week 4: Kronig-Penney model ,Electrons in a periodic potential: Bloch theorem ,Energy bands

Week 5: Numerical methods for energy bands, Fermi surface

Week 6: Semi-classical electron dynamics, Semiconductors and insulators

Week 7: Semiconductors and insulators

Week 8: Two dimensional materials for next generation device applications