

Indian Institute of Technology, Kanpur
Proposal for a New Course

Course No:	CHM6XX
Course Title:	Computational Electronic Structure of Solids
Credits:	3-0-0-0 (9)
Course Duration	Full Semester
Proposing Department/IDP:	Chemistry (CHM)
Departments/IDPs which may be interested in the proposed course:	PHY, MSE, MSP, CHE, ME, EE, AE, SEE
Pre-requisites:	Any one course with fundamentals of quantum mechanics
Proposing Instructor:	Dr. Dasari L. V. K. Prasad

Course Description: This course aims to provide broad understanding of a spectrum of state-of-the-art computational electronic structure methods and tools used in materials science and engineering. Lectures, case studies, demonstrations and hands-on exercises are planned, to provide theoretical and practical knowledge required comprehending the process-structure-property relationships and in aiding the discovery and design of new materials.

#	Topic	# of Lectures
1	Introduction to the course: The gist of relating electronic structure of materials to cohesion, electrical, optoelectrical, mechanical and other various physicochemical properties	02
2	The Basic Approach: Quantum mechanical description of atomic states, molecules and extended solids – the metals and semiconductors	12
3	Unified Electronic Structure Theory for Periodic Systems: k-mesh, Brillouin zone sampling, pseudopotentials, planewave basis set and self-consistent electronic minimizations	10
4	Total Energy and Beyond: Cohesion, modulus of elasticity, States in k-space, phonons, and phase transitions	08

5	Codes and Testing: Linux HPC environment, scripting - coding, graphing, error estimates - uncertainty quantification	02
6	Hands-on Numerical Experiments: Structure description, modeling and simulations of materials – analysis of electronic structure, estimation of forces and force constants, diffusion and mechanical properties	08


Short summary for including in the Courses of Study Booklet:

Chemistry and Physics of Materials; theoretical and computational electronic structure theory; total energy calculations of periodic solid state materials; plane waves and pseudopotential model; Kohn-Sham first principles schemes; tetrahedral solids; zone integrations; band dispersion spectra; lattice vibrations; bulk modulus and elastic constants; numerical high performance computing simulations.

Recommended books/ References:

1. Solid State Theory and Electronic Structure and the Properties of Solids: The Physics of the Chemical Bond, Walter. A. Harrison
2. Solids and Surfaces: A Chemist's View of Bonding in Extended Structures, Roald Hoffmann
3. Atomic and Electronic Structure of Solids, Efthimios Kaxiras
4. Solid State Physics, Neil W. Ashcroft, N. David Mermin and Quantum Theory of Solids, Charles Kittel
5. Reviews and discussions on subject matter will be suggested.

Dated: 18-08-2022


Proposer: Dr. Dasari L. V. K. Prasad

Dated: 21 / 8 / 2022


~~DUGC~~/DPGC Convener

The course is approved / not approved

Chairman, SUGC/SPGC

Dated: _____