

COURSE PROPOSAL UNDER THE MHRD SCHEME GLOBAL INITIATIVE ON ACADEMIC NETWORK (GIAN)

Course Title and Credits

COMPUTATION DESIGN FOR ENERGY APPLICATIONS (1 credit)

Overview

Obama Administration (White House) in US has issued a white paper on Materials Genomic in June, 2011. It says following : Advanced materials are essential to economic security and human well-being, with applications in multiple industries, including those aimed at addressing challenges in clean energy, national security, and human welfare. Accelerating the pace of discovery and deployment of advanced material systems will therefore be crucial to achieving global competitiveness in the 21st century. The Materials Genome Initiative will create a new era of materials innovation that will serve as a foundation for strengthening domestic industries in these fields. This initiative offers a unique opportunity to discover, develop, manufacture, and deploy advanced materials at least twice as fast as possible today, at a fraction of the cost.

The exploration of materials suitable for future energy&pharmaceutical applications continues. Finding a system which can meet certain stringent requirements for energy is one of the challenges for future. In this quest for the ideal energy storage material, first-principles computational tools are heavily utilized to complement experimental studies, characterizing the electronic structure of promising systems or even predicting properties of new materials. The purpose of this course is to provide an overview of the most recent theoretical studies undertaken in the field of materials for energy applications. On selected examples, the application of our computational tool of choice, density functional theory, will be illustrated to show how *ab initio* calculations can be of use in the effort to reach a better understanding of materials and to occasionally also guide the search for new promising approaches.

Objectives

The primary objectives of the course are as follows:

We propose a comprehensive course which will teach how to computationally investigate and design materials first and then on the basis of directions given by novel experimental methodologies, to carry out computational design for new integrated materials. The goal is to reach a comprehensive insight for the design of materials with optimal properties for all of the above applications and utilize this gained understanding to guide the experimental realization and industrial implementation of highly advanced novel materials for humanity.

Course details

Module A: Introduction to Computational Methods

December 26

Lecture 1 : 9:30 to 11:30 AM

DFT, Electronic Structure methods-Solid State methods

Discussion/Tutorial 1: 12:00 noon to 1:00 PM

Module B: Application of Computational Materials Science

December 27

Lecture 2 : 9:30 to 11:30 AM

Hydrogen Storage for Hydrogen Economy

Discussion/Tutorial 2: 12:00 noon to 1:00 PM

December 28

Lecture 3 : 9:30 to 11:30 AM

Materials for Li-ion Batteries

Discussion/Tutorial 3: 12:00 noon to 1:00 PM

December 29

Lecture 4 : 9:30 to 11:30 AM

Hydrogen Production & Fuel cell for Hydrogen Economy

Discussion/Tutorial 4: 12:00 noon to 1:00 PM

December 30

Lecture 5 : 9:30 to 11:30 AM

Materials for Solar cells applications

Evaluation: 12:00 noon to 1:00 PM

Teaching Faculty

Rajeev Ahuja, born in 1965, is Professor of Material Theory at Department of Physics & Astronomy, Uppsala University, Sweden and heads a research group of 17 theoretical physicists. He is one of the most highly cited researchers in Sweden under 50. He has published more than **670** scientific papers in peer reviewed journals (H-Index-**55** & **No. of citations- 13750**), of which 75 are in high profile journals (like Science , Nature , Nature Materials, PNAS , Physical Review letters, Nano Letters , Angew. Chem). Ahuja has been awarded the Wallmark prize for 2011 from KVA (Royal Swedish Academy of Sciences), Stockholm. This award is presented to young scientist (only one scientist every year covering all fields of natural sciences) from King of Sweden. He has previously received the Eder Lilly and Sven Thureus prize and the Benzelius prize from Royal Research Society in Uppsala. Ahuja is an elected member of the Royal Research Society in Uppsala & he on the executive board of the International Association for the Advancement of High Pressure Science and Technology (AIRAPT). Ahuja has supervised 22 PhD students and he regularly acts as a reviewer for several international funding agencies including NSF USA, NRC from Canada, ESF from Estonia, STW from The Netherlands & IBS (100 Milon USD) from South Korea. Ahuja is Panel member and reviewer for Office of Basic Energy Sciences (BES), Office of Science, U. S. Department of Energy (DOE) for Theory, Modeling and Simulation (TMS) at Washington DC. TMS projects are expected to be multi-investigator theoretical efforts with budgets ranging from USD 450,000 to USD 750,000 annually for a 3-year period. He is chief editor of Cogent Physics (Taylor & Francis Group) & editorial board member of Scientific Reports (Nature Publishing Group).

Who can attend?

- Executives, engineers and researchers from manufacturing, service and government organizations including R&D laboratories.
- Student at all levels (BTech/MSc/MTech/PhD) or Faculty from reputed academic institutions and technical institutions.

Registration Fees

Those affiliated to Savitribai Phule Pune University or affiliated colleges: No fee, but registration is must.

Those affiliated to academic and research institutes, NGOs, etc. : Rs. 1000/-

Those from industry: Rs. 5000/-

Those from abroad: US \$ 150

The above fees include tea with biscuits, any instructional material provided by the expert faculty, computer access during any tutorial sessions for the course, wireless internet access via the Savitribai Phule Pune University campus network during the course. Out-station candidates need to arrange for transport and accommodation on their own. 90% or more attendance is necessary to be eligible for an attendance certificate. Appearing for evaluations/examinations during the course is necessary for getting a certificate of grades in the course.

Registration fees is to be paid through a demand draft drawn in the name of Finance and Accounts Officer, Savitribai Phule Pune University, payable at the Pune University Campus Branch, Bank of Maharashtra, Pune 411007.

Host Faculty

[Anjali Kshirsagar](#), Professor and Head
Department of Physics, also at
Centre for Modeling and Simulation
Savitribai Phule Pune University
Pune 411 007 India
Email: anjali@physics.unipune.ac.in, anjali@cms.unipune.ac.in
Web: <http://cms.unipune.ac.in/~anjali/>
Phone: (020) 25692678 ext 200, +91 9850553669

[Sandesh Jadkar](#), Professor
Department of Physics, also at
School of Energy Studies
Savitribai Phule Pune University
Pune 411 007 India
Email: sandesh@physics.unipune.ac.in
Phone: (020) 25692678 ext 415, + 91 9765361124

Local Coordinator :

Saroj Ghaskadbi, Professor
Department of Zoology
Savitribai Phule Pune University
Pune 411 007, India
E-mail : ssg@unipune.ac.in

For any correspondence regarding the course, please send an email to :
gian@physics.unipune.ac.in