COMPUTATION DESIGN FOR ENERGY APPLICATIONS

Course 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.

Dates	**December 26-30, 2016. Maximum Number of participants: 60.**
Who can Attend	Anybody with interest in the course topic and adequate basic training in Physics and Chemistry may attend. Course is designed for student at all levels (BTech / MSc / MTech / PhD) or Faculty from reputed academic institutions and technical institutions or executives, engineers and researchers from manufacturing, service and Government organizations including R&D laboratories. Students with knowledge of quantum mechanics and mathematics and experience with programming will be given preference. Access to a linux-based computer is necessary to perform prototypical calculations. Selection on the first-come-first-served basis after ensuring reasonable background (total capacity: 60; some seats reserved for students from the Savitribai Phule Pune University). Resume/CV with a brief statement of interest/purpose is required for selection and registration.
Fees	**One-Time GIAN Registration:** Visit http://www.gian.iitkgp.ac.in/GREGN/ **Course Fees:** Those affiliated to Savitribai Phule Pune University or affiliated colleges: No fee, but registration is must. Those affiliated to academic institutions, research institutes, NGOs, etc.: ₹1000. Those from industry: ₹5000. Those from abroad: US $ 150. Fees include tea, any instructional material provided by the expert faculty, computer access during any tutorial sessions for the course, internet access via the SPPU campus network during the course. Out-station candidates need to arrange for transport and accommodation on their own. Minimum 90% attendance is necessary to be eligible for certificate of participation/attendance. Appearing for evaluations/examinations during the course is necessary for certificate of grades in the course.

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). Prof. 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). Prof. 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).

Course Coordinator

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GIAN One-Time Registration

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