MATERIALS DESIGNING

Under the aegis of MHRD—Global Initiative of Academic Networks

URL:http://iiti.ac.in/GIAN/

Overview

The comprehensive course will guide researchers to design/investigate materials for novel applications. The purpose of this course is to give 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, which in turn will be very helpful in designing materials for promising applications.

The major goal is to reach an unprecedented 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.

This course has no prerequisite. A student of science with no background in theoretical or computational chemistry knowledge is equally eligible for this course.

The primary objectives of the course are as follows:

- Computational investigation and designing of materials for energy and enviromental application
- The participants will learn to design new integrated materials
- The participants will be introduced to the manifold applications of designed materials with optimal properties as well as gained the understanding to guide the experimental realization and industrial implementation

Schedule of the Course

Schedule of the course : January 04–08, 2018

Total Number of days/lectures : 5 days/10 lectures and 5 tutorials

Registration Fee

Participant from outside India : USD 500

Industry/ Business organization : Rs. 20,000

Academic Institutions : Rs. 1,500

Students : Rs. 1,500

The fee includes all instructional materials, computer use for tutorials, internet facility and lunch. The participants will be provided with accommodation on payment basis.

Topics Covered

The search for materials to address energy, environmental and human welfare related issue is a never-ending process. However, the key is to accelerate the process. Applied computational materials research can play a major role towards accelerating the process. The state-of-the-art first-principles calculations are excellent in predicting properties of new materials. The purpose of this course is to give 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.

Faculty Information

Teaching Faculty

The course will be delivered by Prof. Rajeev Ahuja, Uppsala University, Sweden

Dr. Rajeev Ahuja is a 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 51. He has published more than 750 scientific papers in peer-reviewed journals [H-Index: 57 & citations: 15500 (web of science); H-index: 66 & citations: 20000 (Google Scholar)], of which 80 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. Prof. Ahuja is an elected member of the Royal Research Society in Uppsala & he is an executive board member of the International Association for the Advancement of High Pressure Science and Technology (AIRAPT) & European High Pressure group (EHPRG). Ahuja has supervised 22 PhD students and he regularly acts as a reviewer for several international funding agencies including NSF from USA, NRC from Canada, ESF from Estonia, STW from Netherlands & IBS (100 Million USD) from South Korea. Prof. Ahuja is a 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 a chief editor of Cogent Physics (Taylor & Francis Group) & editorial board member of Scientific Reports (Nature Publishing Group).

Host Faculty

Dr. Biswarup Pathak is an associate professor in the Discipline of Chemistry and Discipline of Metallurgy Engineering and Materials Science at IIT Indore. His major areas of interest are designing of materials for energy and environmental applications. His research area focused on Clean Energy Materials, Hydrogen Production (Photo catalysis) and Hydrogen Production, Li-ion Batteries, Fuel Cell, Surface Catalysis, Molecular Electronics (DNA Sequencing, Molecular Switches). His long-term goal is to establish a centre of excellence in the field of Materials Genome. He has more than 15 years of experience in this field of computational science. Dr. Pathak has published over 90 peer reviewed journal papers in highly reputed international journals. Some of his outstanding works are published in prominent journals such as Journal of American Chemical Society (JACS), Angew. Chem. Int. Ed., Nano Letter, and Journal of Physical Chemistry C (JPCC). In 2016, he has been awarded best researcher at IIT Indore for his outstanding contributions towards materials for energy and catalysis. Recently, he has been awarded Early and Mid-Career Researcher Fellow by Indian National Science Academy (INSA).

Who should attend this course?

1. Executives, engineers and researchers from manufacturing, service and government organizations including R&D laboratories.
2. Undergraduates, MSc, and PhD science stream students. Any student with a basic science background will be able to follow these lectures and gain a lot of insights from them.
3. BSc and MSc level teachers who wish to update their knowledge in frontiers of physics, chemistry and materials engineering.

Course Coordinator

For any further information and registration, please contact:

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