HINDUSTAN UNIVERSITY
HINDUSTAN INSTITUTE OF TECHNOLOGY & SCIENCE

UPPSALA UNIVERSITET

Short term Course On

COMPUTATION DESIGN FOR ENERGY APPLICATION

9 - 11th August, 2017

Organized by: Centre for Clean Energy and Nano Convergence (CENCON), Hindustan University, Chennai

HINDUSTAN UNIVERSITY

Hindustan Institute of Technology & Science (Hindustan University) is a prestigious University accredited with an "A" Grade by NAAC, Govt. of India. QS, the reputed International Rankings Agency has awarded an overall rating of three stars to the University, with a five star rating for Faculty, Employability, Facilities, Innovation and Inclusiveness. Hindustan University has completed over three decades of dedicated service to the nation. It has a cosmopolitan ambience with high-calibre and learned faculty, who are thought leaders, consultants, technology implementers and inventors. The institution is driven by the virtuous vision of the Founder Chairman, Late Dr. K.C.G. Verghese "To Make Everyman a Success and No Man a Failure", and is devoted to the excellence in research, teaching and learning. It lays significant emphasis on quality educational standards that meet demanded of the global workforce, and instills the attitude of life-long learning in the students.

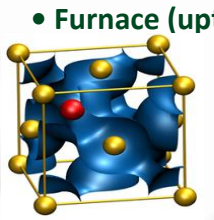
Hindustan University's intense focus on internationalization has led to a long-standing academic collaborations and MoUs with renowned partner institutions and global organizations. The innovative & entrepreneurial spirit of Hindustan community is the driving force behind the evolution of new technologies, products, copyrights and patents that is developed through extensive research carried out at the dedicated Centres of Excellence on campus. The institution has been consistently ranked among the best institutions in the country and aspires to emerge into a global educational institution.

CENCON

CENCON Centre for Clean Energy and Nano Convergence (CENCON), Hindustan University started in collaboration with QSRC, Dongguk University, Korea with a vision to work towards clean energy solutions incorporating the quintessence of Nanotechnology. As a member of the International Consortium on Nanotechnology, the center strives to contribute to the nation's growing need for sustainable energy. As the name goes, an environmental friendly green technology has been developed for the synthesis of nanomaterials and being explored for its various energy applications. A Team of well qualified research scholars in association with International and National expertise from Institutes like Uppsala University, KTH, Sweden, University of Nottingham, Dongguk University, IIT Bombay, IIT Madras, Anna University are working in the following thrust areas: Solar cells, Lithium-ion Batteries, Luminescent devices, Sensors, Photocatalytic applications etc.

The Central Instrumentation Facility (CIF) is a sophisticated Instrumentation Facility of CENCON. The purpose of establishing this center is to provide sophisticated analytical equipment to scientific community. Analytical services are carried out with nominal charges.

- High Performance Computing Cluster with VASP simulation package
- Scanning Electron Microscopy (SEM) with EDAX
- UV – Visible Spectrophotometer with DRS
- Hall Effect measurements
- Spectrofluorometer
- Vacuum thermal coating Unit
- Electrodeposition Unit
- Photoreactor with UV and Visible lights
- Furnace (upto 1200 °C)



OBJECTIVE

In the last few decades, the two terms "energy" and "environment" are extensively being used among the scientific community around the globe. The energy problem is very serious and there is need for developing energy alternatives and R & D in this area. One of the promising options is to make extensive use of renewable sources. The general adoption of sustainable energy technologies depends on the discovery and development of new high-performance materials. The goal of this course is:

- To discuss how first-principles computational methods based on quantum mechanics and statistical physics can drive the understanding, improvement and prediction of new energy materials.
- To learn how the Computation enables to design unprecedented materials of different dimensions with optimal properties and give comprehensive insight for their applications for energy harvesting and storage. The gained understanding would guide the experimental realization and their industrial implementation.
- To learn the density functional theory (DFT), the computational tool and its application to material simulation. Learn to utilize the software like VASP and its application to simulate advance material for energy application.

LECTURES & DEMO BY:

1. Prof. Rajeev Ahuja, Uppsala University, Sweden
2. Prof. Ranjit Nanda, IIT Madras
3. Prof. Rita John, Madras University
4. Prof. Sarat Chandra, IGCAR, Kalpakkam
5. Prof. R. Subramanian, CLRI

DURATION : 3 days (09.08.2017 to 11.08.2017)

WHO CAN ATTEND?

- Faculty , Research scholars & Students (B.Tech./MSc/M.Tech.) of various Colleges and Universities.
- Researchers from Manufacturing, Service and Government organizations including R&D laboratories.

FOCUS & OUTCOME:

The short term course will teach how to computationally investigate and design materials first for energy harvest and storage. Also on the basis of directions given by novel experimental methodologies, computational investigations can be used to design new integrated materials for energy applications.

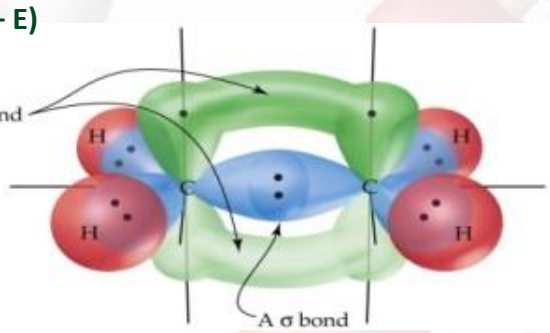
COURSE FEE: Research scholar - Rs.2000 Faculty / Industry : Rs.2500

ACCOMODATION:

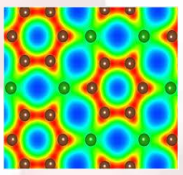
Details pertaining to accommodation available for outstation participants will be intimated soon.

REGISTRATION:

Dr. Puspamitra Panigrahi (SCIENTIST – E)
Email: cencon@hindustanuniv.ac.in
Phone: 044 – 27474262 EXT: 173, 195



Address for Communication:
The Convener, Short term course on CDEA, Centre for Clean Energy and Nano Convergence (CENCON),
Hindustan University, Padur, (OMR), Chennai - 603 103
Phone: +91-44-2747 4262, 2747 4395
Fax: +91-44-2747 4208



Wednesday (09.08.2017)	Resource Person	Topic
9.30 am to 10.45 am	Prof. Rajeev Ahjua	M1: DFT, Electronic Structure methods-Solid State methods
10.45 am to 11.00 am	Break	
11.00 am to 12.00 pm	Dr. Ranjit Nanda	M1: Band Theory and Electronic structure. M2: Materials for Li ion battery D: Setting Up calculations for calculating bandgap for magnetic and non-magnetic systems
12.00 pm to 1.00 pm		
1.00 pm to 2.00 pm	LUNCH	
2.00 pm to 3.00 pm	Dr. Rita John	M1: Band Structure Calculations - a Promising Tool in Materials Investigation • Band Gap Engineering • Impact of transition metal addition • Shape memory alloys and 2D materials investigations
3.00 pm to 3.15 pm	Break	
3.15 pm to 4.00 pm	Dr. Rita John	
Thursday (10.08.2017)		
9.30 am to 10.30 am	Prof. Rajeev Ahjua	M1: Lithium and sodium battery cathode materials: Computational insights
10.30 am to 11.30 am	Dr. Sharat Chandra	M1: Density-functional theory-based study of structural and thermal properties of strongly correlated systems.
11.30 am to 11.45 am	Break	
11.45 am to 12.45 pm	Dr. Sharat Chandra	D: Setting up calculation for total energies as a function of volume
12.45pm to 1.30 pm	LUNCH	
1.30 pm to 2.15 pm	Prof. Rajeev Ahjua	M2: Tuning Hydrogen Storage Desorption Energies: The Crucial Importance of High-Accuracy Calculations
2.15pm to 3.00 pm	Dr. Sharat Chandra	M1: Density Functional Perturbation Theory (DFPT) in conjunction with the quasi-harmonic approximation.
3.00 pm to 3.15 pm	Break	
3.15 pm to 4.15 pm	Dr. Sharat Chandra	D: To set up calculation to calculate the Force Constant.
Friday (11.08.2017)		
9.30 am to 10.30 am	Prof. Rajeev Ahjua	M1: Hydrogen Storage Under High pressure condition.
10.30 am to 11.30 am	Prof. R. Subramanian	M1: Two dimensional materials for sensing application
11.30 am to 11.45 am	Break	
11.45 am to 12.45 pm	Prof. R. Subramanian	
12.45 pm to 1.30 pm	LUNCH	
1.30 pm to 2.30 pm	Prof. Rajeev Ahjua	M2: Enhanced Photovoltaic Performances of 2D materials for Solar cell applications
2.30 pm to 2.45 pm	Break	
2.45 pm to 4.00 pm	Dr. Puspamitra Panigrahi	D: Setting up calculation for evaluation Optical properties

**** M1: Module 1, Introduction to Computation Method.**
M2: Module 2, Application of Computation to Material Science
D: * Partcipants can bring their work (maximum 5 slides) for the discussion with experts