RUKMINI DEVI

Institute of Advanced Studies

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- Category 'A' Institute
- High Grading 81.7% by Joint Assessment Committee of GGSIPU & DHE, Govt. of NCT of Delhi.

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Hands on Training and Workshop-2011 on Computational Methods for Experimental Spectroscopy (Using CASTEP)

Topic :	Hands on Training and Workshop-2011 on Computational Methods for Experimental Spectroscopy (Using CASTEP)
Date of event :	5th-7th January, 2011
Description of the Event :	Eureka! In the pursuit of Science and Technology, RDIAS organized and pulled of with élan a three day mega event on Computational Methods for Experimental Spectroscopy, branch of Physics -providing a mathematical description of much of the dual particle-like and wave-like behavior and interactions of energy and matter. CASTEP is a state of art quantum mechanics based program designed specially for the solid – state materials science. CASTEP can give information about total energies, forces and stresses on an atomic system, as well as calculating optimum geometries, band structures, optical spectra, phonon spectra and much more. It can also perform molecular dynamics simulations. CASTEP uses density functional theory to provide a good atomic-level description of all manner of materials and molecules. CASTEP can give information about total energies, forces and stresses on an atomic system, as well as calculating optimum geometries, band structures, optical spectra, phonon spectra and much more. It can also perform molecular dynamics simulations. In addition CASTEP can be used to study:

	- Total energies.
	- Energies, forces and stresses
	- Electronic structure
	- Charge density, orbital, potentials, band structure, density of states, population analysis
	- Geometry-Optimization of atomic positions and cell parameters with or without constraints and hydrostatic/non – hydrostatic pressure
	- Finite temperatures
	– Molecular dynamics under various constraints and ensembles
	- Transition state searches
	- Phonons – Perturbation theory and finite derivatives, phonon dispersion and density of states, free energy, entropy, heat capacity
	- Electric and Magnetic field responses
	-Polarisability, Dielectric response, NMR spectroscopy, IR and Raman spectra.
	The tutors for this workshop were members of CASTEP Development Group (CDG):
	• **Prof. Stewart Clark**, Professor in Physics, University of Durham, U.K • **Prof. Chris J. Pickard**, Professor at University College, London, U.K • **Dr. Phil Hasnip**, Department of Physics, University of York, U.K • **Dr. Matt Probert**, Senior Lecturer, Physics, University of York, U.K • **Dr. Keith Refson**, Science and Technology Facilities Council, Rutherford Appleton Laboratory, UK.
	It is commendable to note that the previous workshop's were held at:
	• UNIVERSITY OF OXFORD U.K • UNIVERSITY OF YORK • IMPERIAL COLLEGE LONDON
	And now RDIAS would also be included in this distinguished list of host colleges.

Event Report in brief:	This workshop was a three day affair of lectures and laboratory sessions ranging from power of density to NMR methods and Pseudo potentials.
	The event was graced by the esteemed presence of Vice Chancellor, GGSIP University, Prof. Dilip K. Bandyopadhyay who spoke eloquently about the initiative taken by RDIAS towards augmenting research based education and learning. He applauded the efforts of the management in organizing and transforming this idea into reality for the benefit of curious minds. Prof. Bandyopadhyay's zeal for the occasion was exhibited by the fact that he offered a memorandum of understanding to be signed between GGSIP University and the CASTEP Developers Group in pursuit of research interests.
	RDIAS was also witness to its esteemed group of participants from different premier institutes of the country like: IIT Delhi, IIT Chennai, Delhi College of Engineering, University of Hyderabad, Jamia Milia Islamia, BIT Mesra, National Physical Laboratory-Delhi, ABV-IIITM – Gwalior, MPBO- Bhopal, Baba Farid University, Bengal Engineering and Science University-Kolkata, Rukmini Devi Centre of Excellence in Computational Nanotechnology-Delhi, National Environmental Engineering Institute-Delhi, Dr. Hari Singh Gour Vishwavidyalaya-Madhya Pradesh, NIT- Kurukshtra , GGS IP University and GE Global Research, Bangalore.
	This workshop was a mix of scientifically grueling sessions and enjoyable networking through coffee and lunch!
	RDIAS proved to be a warm and caring host for its guests by providing them with comfortable accommodation and catering facilities over the event.
	All the participants were felicitated with participation certificates and a CD each containing the proceedings of the entire session.
	A CASTEP to remember!