Guru Jambheshwar University of Science and Technology, Hisar
Organizes One Week
GIAN-MHRD, Government of India Sponsored Workshop-Course
On
"NANOTECHNOLOGY: Insights into properties of materials from Computational Modeling Methods"
(From 16th Oct, 2016 to 20th Oct, 2016)

Overview

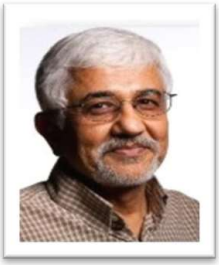
Nanotechnology is a technology that relies in the regime between one to hundred nanometers, viz. billionths of the meter. In this course, students will learn about computational modeling methods which are being used to gain insight into properties of materials for applications in nanotechnology. For example, discovery of carbon related nanostructures including fullerene, nanotubes and graphene have sparked an extraordinary amount of research activities on their unique properties and novel applications in electronics and optoelectronics. However, the gapless nature of graphene is one of the import obstacles for its applications in transistors. This is now being addressed by computer modeling methods together with experimental methods. In this course, the students will learn about quantum chemical methods based on density functional theory to determine structural, mechanical, electronic and optical properties of materials at nanoscale. Also, the students will learn how to simulate and characterize device configuration based on nano materials. The course will be planned and offered as per the norms set by Guru Jambheshwar University of Science and Technology.

Modules	**Module A: Nanotechnology and Computational Modeling Methods** **1. October 16, Sunday** **Inauguration:** 9:00 AM a. **Lecture 1:** 9:30 to 10:30 AM Introduction to nanotechnology b. **Lecture 2:** 10:45 to 11:45 AM Introduction to materials c. **Tutorial 1:** 2:00 to 4.00 PM Problem solving session with examples **2. October 17, Monday** a. **Lecture 3:** 9:30 to10:30 AM Introduction to methods in modeling of materials b. **Lecture 4:** 10:45 to11:45 AM Introduction to methods in modeling of materials c. **Tutorial 2:** 2:00 to 4.00 PM Problem solving session with examples

	3. October 18, Tuesday a. **Lecture 5:** 9:30 to 10:30 AM Recapitulating Nanotechnology and Computational modeling b. **First Exam for Participants** : 11:00AM to 12:30 AN **Module B: Device characteristics** **4. October 19, Wednesday** a. **Lecture 6:** 9:30 to10:30 AM Introduction to electronic devices b. **Lecture 7:** 10:45 to 11:45 AM Introduction to theory of electron transport c. **Tutorial 3 :** 2:00 to 4 PM Problem solving session with examples **5. October 20, Thursday** a. **Lecture 8:** 9:30 to 10:30 AM Recapitulating Device characteristics b. **Second and Final Examination** : 10:45AM to 12:15 AN **c. Valediction :** 2:00 PM to 2:30 PM **Number of participants for the course will be limited to fifty.**
You Should Attend If…	• Executives, engineers and researchers from manufacturing, service and government organizations including R&D laboratories. • Student at all levels (B.Tech/M.Sc./M.Tech./Ph.D) or Faculty from reputed academic institutions and technical institutions.
Fees	**The applicant are required to get themselves register on GIAN web portal (http://www.gian.iitkgp.ac.in) to apply for any number of GIAN courses as and when necessary.** The course registration fee is separate. The participation fees **(Demand draft drawn in favour of Registrar, GJUS&T, Hisar or NEFT/RTGS at PNB A/c No.** 4674000100036542 IFSC : PUNB0467400**)** for taking the course is as follows: **Participants from abroad : US $500** **Indian Industry/ Research Organizations: Rs. 2,000** **Indian Academic Institutions: Rs. 1,000** The above fee includes all instructional materials, computer use for tutorials and assignments, laboratory equipment usage charges, 24 hr free internet facility. The participants will be provided with accommodation on payment basis, subject to availability.

The Faculty

Foreign faculty



Ravindra Pandey is Professor and Chair of Physics at the Michigan Technological University, Houghton, MI. Pandey received his education at Hari Singh Gaur University, Sagar, National Physical Laboratory, Delhi, Atomic Energy Research Laboratory, Harwell, UK and University of Manitoba, Winnipeg, Canada. He has participated in multi-disciplinary efforts (theoretical and experimental) to build the programs in novel nanostructures, and application of chalcopyrite semiconductors as the next generation optoelectronic materials with the industrial and national laboratories, and is the author of more than 150 publications. He has also co-organized and participated in several international conferences in the areas of Materials Physics and Nanoscale Science. Pandey is Fellow of American Physical Society.

Host faculty

Dr. Tankeshwar is Vice Chancellor of Guru Jambheshwar University of Science and Technology. He did his M.Sc and Ph.D(1990) in Physics from Panjab University, Chandigarh. He did his post-doctorate research at International Centre of Theoretical Physics, Italy in the year 1990-91. He has worked at Panjab University as UGC Professor. The work done by Dr Tankeshwar over nearly two and a half decades makes distinct contributions to understanding of transport phenomena which finds numerous applications in various branches sciences. His scientific contribution to transport properties of liquids and fluid confined to different nano-geometries. Several exact sum rules have been derived for various dynamical time correlation functions. One of important contributions is to show that confinement at nano length scale results in local and anisotropic diffusion.

Course Co-Coordinator

Dr. Sandeep Kumar, Assistant Professor, is a researcher of international recognition at the Department of Bio and Nano Technology, Guru Jambheshwar university of Science and Technology, Hisar, Haryana, India. His research areas include synthesis and characterization of nanomaterials, nanocarriers for healthcare applications, nanomaterials based sensors, biomaterials and nanotoxicology. He has one patent and published more than 50 research papers in international journals of repute. Dr Kumar has international and national sponsored research projects from different funding agencies like DST, DBT, DRDO etc. He visited Hanyang University, Seoul, South Korea as a visiting Professor and also Australia, UK, Scotland, Bangkok under different schemes of Govt of India.

Course Co-ordinator

Prof. Tankeshwar Kumar
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List of Participants

S. No.	Name	Affiliation	Institute/University
1.	ABHINAV NAG	PH.D. SCHOLAR	DEPT. OF PHYSICS, CENTRAL UNIVERSITY OF HIMACHAL PRADESH, KANGRA, HIMACHAL PRADESH
2.	AKANKSHA SOOD	PH.D. SCHOLAR	DEPT. OF CHEMISTRY, PU, CHANDIGARH
3.	AKARITI SHARMA	PH.D. SCHOLAR	DEPT. OF PHYSICS, PUNJABI UNIVERSITY, PATIALA, PUNJAB 147002
4.	AMRISH SHARMA	PH.D. SCHOLAR	DEPT. OF BASIC AND APPLIED SCIENCE, PUNJABI UNIVERSITY, PATIALA, PUNJAB 147002
5.	ANAND KUMARI	PH.D. SCHOLAR	DEPT. OF PHYSICS, GJUS&T, HISAR
6.	ANISHA	M.Sc. STUDENT	DEPT. OF BIO AND NANO TECH, GJUS&T, HISAR
7.	ANITA YADAV	PH.D. SCHOLAR	DEPT. OF PHYSICS, IIT ROPAR RUPNAGAR PUNJAB 140001
8.	ANJNA DEVI	PH.D. SCHOLAR	DEPT. OF PHYSICS, HIMACHAL PRADESH UNIVERSITY, SHIMLA
9.	ANKUSH BHARTI	PH.D. SCHOLAR	DEPT. OF PHYSICS, HIMACHAL PRADESH UNIVERSITY, SHIMLA
10.	ANU GUPTA	FACULTY	SETH JAI PRAKASH MUKAND LAL INSTITUTE OF ENGG. & TECH., RADAUR, YAMUNANAGAR
11.	ANUJA KUMARI	PH.D. SCHOLAR	DEPT. OF PHYSICS, CENTRAL UNIVERSITY OF HIMACHAL PRADESH
12.	ANURAG	FACULTY	GJUS&T, HISAR
13.	ASHUTOSH KUMAR SHAHI	RESEARCH ASSOCIATE	DEPT. OF PHYSICS, IIT BHU
14.	AWADHESH KUMAR VERMA	PH.D. SCHOLAR	JAMIA MILLIA ISLAMIA, NEW DELHI
15.	DALJOT SINGH KANG	STUDENT	PU, CHANDIGARH, 160014

16.	DEEPAK KEDIA	FACULTY	DEPT. OF ECE, GJUS&T, HISAR
17.	DEEPAK KUMAR DINKAR	M. TECH STUDENT	DEPT. OF MATERIALS SCIENCE & NANOTECH., DCRUST, MURTHAL, HARYANA
18.	DEEPIKA	PRE-DOCTORAL FELLOW	DEPT. OF PHYSICS, IIT ROPAR, RUPNAGAR, PUNJAB
19.	DEOBRAT SINGH	PH.D. SCHOLAR	DEPT. OF APPLIED PHYSICS, SVNIT, ICHCHHANATH, SURAT
20.	DHANANJAYA PANDA	PH.M STUDENT	DEPT. OF PHYSICS, AISECT UNIVERSITY, BANGRASIA, BHOPAL
21.	EKTA ARYA	PH.D. SCHOLAR	DEPT. OF PHYSICS, GJUS&T, HISAR
22.	GEETA SACHDEVA	M.Sc. STUDENT	CENTRAL UNIVERSITY OF PUNJAB
23.	GUR SIMRAT KAUR	PH.D. SCHOLAR	DEPT. OF PHYSICS, PU, CHANDIGARH
24.	KAPILA TANEJA	PH.D. SCHOLAR	DEPT. OF BIO & NANO TECH, GJUS&T, HISAR
25.	KESHAV DEV	FACULTY	DEPT. OF PHYSICS, R. S. GOVT. P.G., COLLEGE, LALITPUR
26.	KUMAR SAURABH YADAV	PH.D. SCHOLAR	DEPT. OF PHYSICS, BUNDELKHAND UNIVERSITY, JHANSI, U.P.
27.	KULVEER KAUR	PH.D. SCHOLAR	DEPT. OF PHYSICS, PUNJABI UNIVERSITY, PATIALA
28.	MANJEET KUMAR	PH.D. SCHOLAR	DEPT. OF MECHANICAL ENGG., PU CHANDIGARH
29.	MANISHA	PH.D. SCHOLAR	DEPT. OF PHYSICS, GJUS&T, HISAR
30.	MEENAL	PH.D. SCHOLAR	DEPT. OF PHYSICS, GJUS&T, HISAR
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33.	MOONDEEP CHAUHAN	PH.D. SCHOLAR	DEPT. OF ENVIRONMENT STUDIES, PU, CHANDIGARH

34.	MUKHTIYAR SINGH	FACULTY	DEPT. OF PHYSICS, DAYANAND COLLEGE, HISAR
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36	MUSKAAN TUTEJA	PH.D. SCHOLAR	DEPT. OF PHYSICS, GJUS&T, HISAR
37.	NAVEEN KUMAR	FACULTY	SHOOLINI UNIVERSITY, SOLAN
38.	NAVJOT MEHTA	M.TECH STUDENT	DBNT, GJUS&T, HISAR
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43.	PARAMJEET	RESEARCH ASSOCIATE	NPL, NEW DELHI
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48.	PRABAL DEV BHUYAN	PROJECT FELLOW (DST PROJECT): STUDENT	DEPT. OF PHYSICS, ST. XAVIERS COLLEGE, AHMEDABAD,GUJARAT
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58.	RUMA RANI	PH.D. SCHOLAR	DEPT. OF BIO. & NANO TECH, GJUS&T, HISAR
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63.	SHIVANI KAPOOR	PH.D. SCHOLAR	DEPT. OF BIO. & NANO TECH, GJUS&T, HISAR
64.	SOURAV SINGLA	ME STUDENT	UIET, PU, CHANDIGARH
65.	SUMANDEEP KAUR	PH.D. SCHOLAR	DEPT. OF PHYSICS, PU, CHANDIGARH, 160014
66.	SUNITA SRIVASTAVA	FACULTY	DEPT. OF PHYSICS, PU, CHANDIGARH, 160014
67.	SUSHILA DEVI	PH.D. SCHOLAR	DEPT. OF PHYSICS, HIMACHAL PRADESH UNIVERSITY, SHIMLA HIMACHAL PRADESH 171005
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77	JOGENDER SINGH	PH.D. SCHOLAR	DEPT. OF PHYSICS, GJUS&T, HISAR
78	RITESH KUMAR	PH.D. SCHOLAR	DBNT, GJUS&T, HISAR

GIAN

Global Initiative of Academic Network (GIAN) Programme
Guru Jambheshwar University of Sc. & Tech Guru Jambheshwar University of Sc. & Tech.

Report on Conduct of GIAN Course

Course Title	NANOTECHNOLOGY: Insights into Properties of Materials from Computational Modeling Methods
GIAN Course ID	166016M01
Period of Course	From 2016-10-16 To 2016-10-20
Name and Department of Faculty from IIT Kharagpur Course Coordinator	
Name	DR. TANKESHWAR KUMAR
Department	VICE-CHANCELLOR, GURU JAMBHESHWAR UNIVERSITY OF SCIENCE AND TECHNOLOGY
Co-host Faculty, if any	
Name	
Department	
Name and Affiliation of International Faculty	
Name	PROF. RAVINDRA PANDEY
Department	Professor Ravindra Pandey, USA
Name and Affiliation of national Faculty	
Name	1.) DR. TANKESHWAR KUMAR; 2.) DR. SANDEEP KUMAR;
Department	1.) VICE-CHANCELLOR, GURU JAMBHESHWAR UNIVERSITY OF SCIENCE & TECHNOLOGY 2.) ASSISTANT PROFESSOR, DEPT. OF BIO AND NANO TECHNOLOGY, GURU JAMBHESHWAR UNIVERSITY OF SCIENCE & TECHNOLOGY
Structure of the Course	
Duration of Course(1 Week or 2 Weeks)	1
Number of credits	1
Total number of lectures in the course	10
Number of lectures by International Faculty	10
Number of lectures by Host Faculty	
Number of hours of laboratory/tutorial sessions	08
Participants of the Course	

Number of Student participnats	66
Number of participnats from Industry/Research	
Number of faculty participnats	12
Total Number of Participants	78
Number of participnats who credited for the course	78
Course Generated Fund	
Sponsorship. if any (in Rs)	
Registration Fee Collected	77000
Total Amount	77000
Interaction with International Faculty	
Interaction of Host Faculty	There was a very warm interaction of host faculty with international faculty. The workshop day started with the reporting process of participants with diverse fields of specialization and from different educational institutions of India including IIT Ropar, IIT BHU, Jamia Millia Islamia, Panjab University Chandiagrh, HPU Shimla, Bundhelkhand University, Jhansi, Central University of Gujrat, Central University of Himachal Pradesh etc. After completion of initial documentary formalities, Course coordinators Professor Tankeshwar Kumar welcomed all the participants with smile and ensured comfortable environment for everyone in the new setting. There was a very warm interaction of host faculty with international faculty. Dr. Tankeshwar Kumar introduced Prof. Ravindra Pandey, Prof. Loredana Valenzano and Dr. Ashok Kumar to all the participants. He mentioned the vision and purpose of GIAN workshop. He suggested and asked all participants to get answers to all their queries about different aspects of their research work during this workshop-course. Prof. Ravindra Pandey explained beautifully the power of First Principles Methods. He gave some tips to the young researchers and advised them to formulate the problem first of all, and then choose the model (LDA -> GGA -> vdW) for the problem and motivated participants to be aware of available computational resources like SIESTA, Quantum Espresso and Gollum. He also asked the participants to prepare 'one ppt' summary every week – "progress" and read scientific literature (10 mins reading of a paper every day).
Interaction of other faculty from Guru Jambheshwar University of Sc. & Tech	Dr. Sandeep Kumar gave a warm welcome to all international/national experts and also thanked for giving their valuable time to this workshop-course. He interacted with all faculties and participants from different institutes/organizations, and thanked to all for becoming part of this workshop-course. Other faculties of GJUS&T Hisar e.g. Dr. Vikas Verma, Dr. Ramesh Kumar, Dr. Hardev Singh, Dr Deepak Kedia, Dr Santosh Kaushik, Dr Neeraj Dilbaghi and some other new faculties of the institutes interacted with the experts and the participants of the workshop. The faculty members became more knowledgeable, got benefited from this event and obtained new ideas to gear up their research career in frontier areas of science and technology.

Interaction of faculty /researchers from other institutes/organizations	The interaction of faculty/researchers from other institutes/organizations was very good. The participants came from the various reputed educational and research institutions throughout India such as HPU, Shimla, IIT, Ropar, PU, Chandigarh and many more. There were extreme diversity among participants and they very excited to learn computational studies of nanomaterials from international/national faculty. During this workshop Prof. Ravindra Pandey delivered lectures and interacted with participants during tutorial sessions along with Prof. Loredana Valenzano and Dr. Ashok Kumar. Prof Pandey shared various burning research fields such as CNT, MOFs, electrons transfer at nanoscale and Tuning Electronic Properties of 2D Material for Device Applications etc which have large practical applications. Payal wadhwa group from IIT, Ropar asked about the polymer plotting in different dimensions and discussed accuracy of the approach for the particular problem. Preeti from the same group asked many questions regarding the low dimensions systems such as graphene, CNT etc. Abhinav Nag group from HPU, Shimla was working on quantum dots. They asked about the toxicity of CdSe at nanoscale and whether core-shell structure has the possibilities to overcome the toxicity of a core material or not. Dr. Ramesh Kumar form GJUS&T Hisar asked queries related to the modelling of the nanomaterials during lecture as well as hands on session. Many queries were taken by Prof. Pandey from the participants and almost all the participants resolved their research related problem and got new ideas for research. The participants were very excited in the tutorial session to learn electronic structure calculations on Quantum Espresso software. Prof. Ravindra Pandey, Dr Ashok Kumar and Dr Hardev Singh took all queries from all participants regarding commands of LINUX operating system. Participants learnt Basic Linux Commands, Simple SCF Calculations of bulk Si, Surface Calculations of-Al (001), Acetylene (C_2H_2) etc. Every participant run the total energy calculations and calculated the some ground state properties such as bulk modulus, Equilibrium lattice constant, DOS and band structure etc of the basic materials. Dr Ashok Kumar, Dr Loredana and Dr. Hardev Singh helped them to create the input file and Visualization of structure in the sample input file using Xcrysden. Among all participants, faculty members (Deepak Kedia, Santosh Kumari, Ramesh Kumar, Vikash Verma, Anurag etc.) were present to learn the new areas/fields in nanotechnology in their respective fields. Dr. Deepak Kedia asked about measurement of strain applied to a crystal manually. Dr. Vikas Verma discussed various problems with Prof. Loredana Valenzano and tried to learn the role of DFT calculations in the inorganic chemistry.
Signature of Course Coordinator	
Date of submission of report	