

Report on

One week FDP on “Computational Modelling of Materials” (online mode) May 08th to May 12th, 2023

Conducted by

Department of Physics



FACULTY DEVELOPMENT PROGRAM
On
Computational Modelling of Materials

Title
Interplay of Electrical and Thermal Conductivities to enhance Thermoelectric Performance for Device Applications

Dr. Raju Kumar Biswas
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Raju K Biswas
Dr Sreedhar S
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Report submitted by: **Dr. Sunku Sreedhar, Assistant Professor, Department of Physics,**

Conveners: **Dr. Md Mahabul Islam, Dr. Sunku Sreedhar, and Dr. Usuf Rahaman**

About FDP cum workshop theme:

The conference theme is computation modeling of materials. It includes modeling of various materials using Density Functional Theory (DFT) methods using quantum mechanical toolbox. These unique computer simulations have the wide capabilities such as modeling of new kind of materials, predicting the materials behaviors, tuning and insight valuable information of characteristics, bandgap, spectroscopy of materials can prediction/analyze etc. could be done. *DFT based quantum mechanical simulations were a revolution in material science. Nowadays it is widely used by researchers from different fields to explore innovative materials and validate their behaviors prior to the manufacturing.*

About Registration:

We got “**blockbuster response of 1286 registration across the globe**”. The brochure and registration link shared to various active groups belonging to academic and research. In short notice we got a tremendous response as registrations crossed 1200 (one thousand two hundred) before the start of the conference. This gives us good motivation and starting the FDP with high energy. The various types of audience like research scholars, early carrier researchers, young faculty, experienced people shown interested to learn and explore about latest developments in DFT quantum mechanical simulations.

The program is scheduled as given below with the list of speakers. Each day two eminent speakers from reputed institutions like IISER, IITs, and other reputed institutions who have very good and proved experience in the computer simulations of materials were selected to deliver lectures. Each talk has limited to 1-hour to 2-hour duration including discussions.

Country	No. of Participants registered
INDIA	1251
Algeria	1
Australia	1
Bhutan	1
China	3
Colombia	1
Côte d'Ivoire	1
Colombia	2
Malaysia	1
Morocco	7
Nepal	1
Nigeria	1
Oman	1
Pakistan	10
SOUTH KOREA	1
UAE	1
Uganda	1
ZAMBIA	1
Total	1286

Program Schedule

S. No.	Speaker Name	Title of the talk	Date and Time
		Inauguration of FDP	08 th May 2023, 10:30 am
1	Dr. Bheemalingam Chittari, IISER Kolkata	Quantum theory of functional materials: energy storage, magnetism, and superconductivity.	08 th May 2023, 11:00 am -12:30 pm
2	Dr. Raju Kumar Biswas, Ramaiah University of applied Science, Bangalore, India	Interplay of electrical and thermal conductivities to enhance Thermoelectric Performance for device applications	08 th May 2023, 15:00 pm-16:30 pm
3	Dr. Soumyasree Jena, NIT Raurkela	Study of multi-functional materials using first-principle methods	09 th May 2023, 11:00 am-12:30 pm
4	Dr. Kulwinder Kaur, Mehr Chand Mahajan DAV College for Women, Chandigarh.	Thermoelectric Materials and Their Emerging Applications	09 th May 2023, 14:30 pm-16:00 pm
5	Dr. G. Shwetha, Anurag University, Hyderabad	High pressure structural phase transition of Sc-based ternary Borides from first-principle calculations	10 th May 2023, 14:00 pm-15:30 pm
6	Prof. Akhilesh Tiwari, IIIT Allahabad, Prayagraj, Uttar Pradesh	Modeling and Simulation: A case study of Photonic Crystal Metamaterials.	10 th May 2023, 15:30 pm-17:00 pm
7	Dr. Rajibul Islam, University of Alabama at Birmingham,USA	Discovery of quantum materials using ab-initio study	11 th May 2023, 10:30 am -11:30 am
8	Dr. Debolina Misra, IITDM, Kancheepuram, Chennai, India	Rational Design of Single Atom Catalysts from First-principle Calculations.	11 th May 2023, 14:00 pm -15:30 pm
9	Dr. Ravi Kashikar, University of South Florida, USA	Electronic structure of Halide perovskites.	12 th May 2023, 10:00 am -11:30 am
10	Mr. Ahmed Syed, IIT Madras, Chennai.	Collective Dynamics and Evacuation: Modeling and Experiments in Human Crowds	12 th May 2023, 14:30 pm-16:00 pm
11.		Group photo session, Valedictory	12 th May 2023, 14:30 pm-16:00 pm
12.		QUIZ and feedback	12 th May 2023, 16:00 pm-17:00 pm

Day 1: 08-05-2023 (Monday)

The program commenced at 10.30 AM with a welcome note by **Dr. M. Chandra Sekhar**, Head, Department of Physics, **MITs**, and coordinator for the conference. He elucidates about the departmental activities and research activities details going in the department of physics and **Vice principal, Prof. P. Ramanathan** Presented Inaugural address to audience. **Dr. Eswar S**, **CSO** of **MITs**, addressed the audience and highlighted the concept of making FDP online mode for the usefulness to the research community. **Dr. Md Mahabul Islam** address the gathering and aim scope of thematic conference and details about the speakers in the conference. **Dr. Sunku Sreedhar** presented the gathering about the structure of the FDP and criteria of obtaining FDP, such as quiz, feedback submission etc.

Welcoming to the first speaker of FDP cum workshop **Dr. Bheemalingam Chittari**, from **Indian Institute of Science Education and Research (IISER) Kolkata**. He is a prominent scientist with 18 years of research experience in the field of modeling and simulation of materials. He published research papers in very high impact journals like Nature Materials, Nature communications, Physical Review Letters etc.,. He delivered the first talk on Quantum theory of functional materials and explained the modeling and simulations of superconductivity, and energy storage materials. He outlined modeling of a few complex structures like graphene based heterostructures, more lattice structures using quantum mechanical simulations.

The second Session started on the same day afternoon **Dr. Raju Kumar Biswas**, **Ramaiah University of applied Science, Bangalore, India** explained about simulating of thermoelectric materials and how the performance can be validated for device applications and interplay of electrical and thermal conductivities to enhance the performance of these materials.

Day 2: 09-05-2023 (Tuesday)

On the second day the first half of the talk from 11.00 am to 1.00 p.m. is given by **Dr. Soumyasree Jena**, **NIT Raurkela**, she outlined the Study of **Multi-Functional Materials using First-Principle Methods**. The talk consists of the study of various properties for the heterostructure thin films using quantum mechanical computing techniques.

The afternoon session started at 2.30 pm and continued upto 4.00 pm is given by **Dr. Kulwinder Kaur, Mehr Chand Mahajan DAV College for Women, Chandigarh**. She discussed various computational techniques involved in exploring the **Thermoelectric Materials Figure of Merit Estimations**. How one can choose novel material by using computer simulations.

Day 3: 10-05-2023 (Wednesday)

The third day both the sessions conducted in the afternoon only based on convenience of the speakers, first talk form 14.00 pm to 15.30 pm is scheduled by **Dr. G. Shwetha, Anurag University, Hyderabad**, High pressure structural phase transition of Sc-based ternary Borides from first-principle calculations. She given valuable overview of different software tools based on quantum mechanical simulations. It is useful to identify for the particularly solving the task.

The second talk is given by **Prof. Akhilesh Tiwari, IIIT Allahabad, Prayagraj, Uttar Pradesh** given exciting talk of Modeling and Simulation: A case study of Photonic Crystal Metamaterials using COMSOL Multiphysics simulations. An extensive study on photonic materials, optical fibers, etc. simulations are provided.

Day 4: 11-05-2023 (Thursday)

The fourth day first talk is given by **Dr. Rajibul Islam, University of Alabama at Birmingham, USA**. He told in his talk Discovery of quantum materials using ab-initio study. The afternoon session the talk given by **Dr. Debolina Misra, IITDM, kancheepuram, Chennai, India**, Her talk is Rational Design of Single Atom Catalysts from First-principle Calculations.

Day 5: 12-05-2023 (Friday)

The Final day the first session on morning commenced by **Dr. Ravi Kashikar, University of South Florida, USA**, A very exciting talk on **Electronic structure of Halide perovskites** is given in the morning 10.00 am to 11.30 am. A detailed overview of quantum mechanical calculations of different halide materials was discussed.

The second session an interesting out of the box talk given by **Mr. Ahmed Syed, IIT Madras, Chennai**. The talk is on **Collective Dynamics and Evacuation: Modeling and Experiments in Human Crowds**, the essential simulation study very useful to make protocols for crowd management to avoid death of people in overcrowded zones.

Day 5: 12-05-2023 (Friday) Group photo session, Valedictory

The valedictory session is handled by **Dr. M. Chandra Sekhar**, Head, Dept. of Physics, **Vice principal, Prof. P. Ramanathan** presented valedictory address to audience and vote of thanks given by **Dr. B. Jagadeesh Babu**, Dept. of Physics, MITS. It flowed by QUIZ time for participants to qualifier for getting certificate.

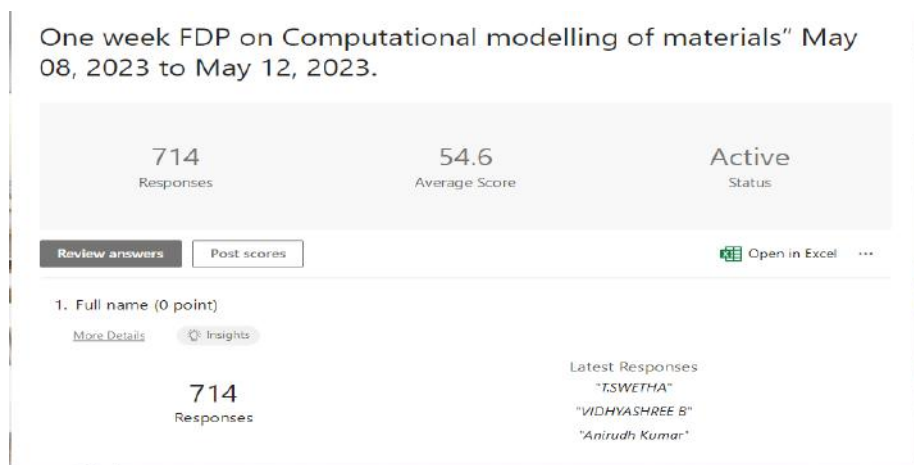
The final Quiz is attempted by 716 participants out of 590 eligible participants issued an FDP cum Workshop certificates.

We thank all eminent speakers whose involvement is highly appreciated. All of them deliver excellent material which is very useful for the research community. Without the contributions of speakers, the FDP may not be a grand success. The best part is all the speakers given a presentation with no remuneration as we are conducting free for all the participants. The wide presence of active participation from various institutions throughout the workshop is highly appreciated. We thank all the active participants for their participation. We thank valuable support from technical support from systems, MITS, all other faculty, and well-wishers who are not mentioned in this list.

We thank Principal sir, Prof. C. Yuvaraj and Vice Principal, Prof. P. Ramanathan for his cooperation during the FDP.

Our heart fell thanks to the management, MITS Madanapalle, for encouraging and supporting us.

The number of participants attending the FDP workshop

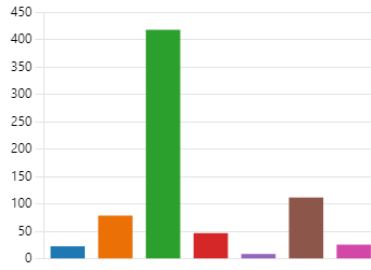


The various categories of participants from different institutions.

5. Designation (0 point)

More Details Insights

- Professor 23
- Associate Professor 79
- Assistant Professor 418
- Lecturer 47
- Post Doctoral Student 9
- Doctoral Student 112
- UG/PG Student 26



6. How do you rate the conference topics related to Computational modeling (0 point)

More Details Insights

Snippets

The screenshots are from a Zoom meeting titled "One week FDP on Computational modelling of materials * Day1 Dr. Bheemlingam Chittari".

Slide 1: Hearty Welcome
 One week Faculty Development Programme on "Computational Modelling of Materials" May 08, 2023 to May 12, 2023. (Online Mode)

Slide 2: Resource Persons

Dr. Bheemalingam Chittari Indian Institutes of Science Education and Research, Kolkata. Dr. Raju Kumar Biswas Ramalah University Bangalore. Dr. Soumyasree Jena National Institute of Technology, Rourkela. Dr. Kulwinder Kaur Mehw Chand Mahajan DAV College for Women, Chandigarh.	Dr. Ahmed Syed IIT Madras, Chennai. Dr. G Shwetha Anurag University, Hyderabad. Dr. Rajbul Islam University of Alabama at Birmingham. Dr. Debolina Misra IITDM Kancheeppuram, Chennai. Dr. Ravi Kashikar University of South Florida.	Prof. Akhilesh Tiwari Indian Institute of Information Technology Allahabad, Prayagraj, Uttar Pradesh.
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Slide 3: Speaker

Dr. Bheemalingam Chittari
 Indian Institute Of Science Education And Research Kolkata, Kolkata.
Title of the talk : Quantum theory of functional materials: energy storage, magnetism, and superconductivity
 Day 1: 08th May 2023, 11:00 am -12:30 pm