

**International Workshop on Experimental and Simulation Solution for Developing Novel Sustainable Materials,  
FEBRUARY 08-10, 2023**

**Report**

An International Workshop on “Experimental and Simulation Solution for Developing Novel Sustainable Materials” was organized by DEPARTMENT OF PHYSICS GOVT. NAGARJUNA P.G COLLEGE OF SCIENCE RAIPUR, CHHATTISGARH, INDIA Sponsored by CHHATTISGARH COUNCIL OF SCIENCE AND TECHNOLOGY RAIPUR, CHHATTISGARH, INDIA

The workshop aims at the following objectives: • To exchange the latest state of the art scientific information in the field of Computational Material Science and Nanotechnology. • To provide a platform to the participants for exchanging the knowledge and viewing the international scenario by interacting with senior scientists of international repute. • To establish a working relationship and to explore the future research prospects by way of inter-institutional collaborations.

A three days international workshop on EXPERIMENTAL AND SIMULATION SOLUTION FOR DEVELOPING NOVEL SUSTAINABLE MATERIALS (IWESSM 2023) was organized by Department of Physics, Govt. Nagarjuna PG College of Science Raipur Sponsored by CGCOST on blended mode. Some students and Faculty members from this college and from nearby colleges attended the workshop at E-classroom of college.

Before starting the workshop, on 7/2/23 a special session (pre installation) was arranged for SIESTA software installation and introduction about the Simulation process. This session was taken by DR. Mohan L Verma and Narendra Kumar at 11:00 AM To provide Online Platform to the participants of this workshop a Zoom subscription has been purchased for one month (4<sup>th</sup> Feb 23 to 3<sup>rd</sup> Mar 23) and a YouTube channel, Facebook page and whatsapp Group was also created by Department of physics.

Day-1, 08.02.2023 (Inaugural Function)-

The IWESSM 2023 was inaugurated at 9:30 am in the morning at Department of physics of Government Nagarjuna Post Graduate College of Science by worshipping goddess Saraswati. All Dignitaries were welcomed Prof. Anjali Oudhia HoD of the Department of Physics (Chairperson) gave the welcome Address and the Introduction of first day of program. Prof. Oudhia welcomed all the dignitaries, the resource persons, faculties and research scholars joined the virtual Workshop from various universities and institutes. She congratulated all the members of organizing committee for organizing the Workshop. At the inauguration ceremony prof. Raveindra Pandey, Prof Physics, Michigan Tech University USA: Prof Namita Brahme, HOD Physics Pt. RSU, Raipur, Dr. D.P. Bisen, SoS Physics Pt. RSU, Raipur Dr. Mohan L Verma, SSTC, Bhilai, were also present.

In this Workshop on our call 130 participants have registered from 7 different states of the country. The program was conducted in seven different sections namely, Inaugural function, Technical session-1, technical session-2, technical session-3, and three hands on sessions.

Dr Namita Bramhey of HoD SoS Physics, Pt Ravishankar University was anointed as chairperson of the inaugural session. She introduced Prof. Ravindra Pandey from Michigan Tech University, USA (Key Note Speaker) Keynote Speaker Prof. Ravindra Pandey from US gave insight about Computational Methods in Research field and its importance in simulation. Prof Namita Bramhey gave vote of thanks to Prof Ravindra Pandey after his session.



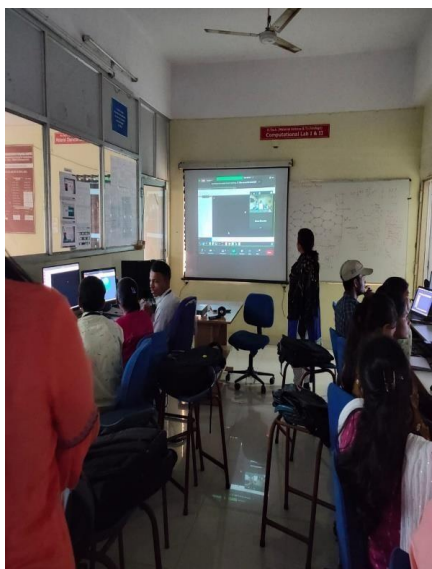
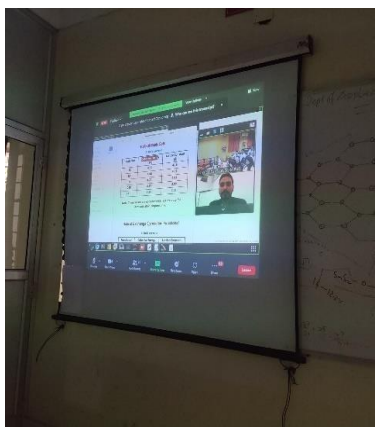
Principal of Government Nagarjuna Post Graduate College of Science Prof. P. C. Choubey felicitated Prof Ravindra Pandey and all other guests.

### **Technical Session-1 (11:30 am-1:00 pm) -**

In the first technical session there were two talks (one invited and one Plenary ). Dr. Milind Rane joined from IIT Mumbai for invited talk .He talked about Novel use of Plastic in Solar Materials. Dr. B Verma gave Vote of Thanks at this note.

Plenary Talk was given by Dr Rodrigo of Brazil and he Explained DFT (Density Functional Theory) at a fundamental level. Prof. Sameer Thaker gave vote of thanks.

**Hands on Session -1 (3:00 pm -5:00 pm)** A Hands On Session in second half of the program was taken by Dr. Mohan L Verma SSTC ,Bhilai and Dr Narendra Bansal of Abu Dhabi. The session dealt with various commands of Siesta and fdf file downloading, that is very much helpful in computing characteristics of any molecule.



**Day -2, 09/02/2023**

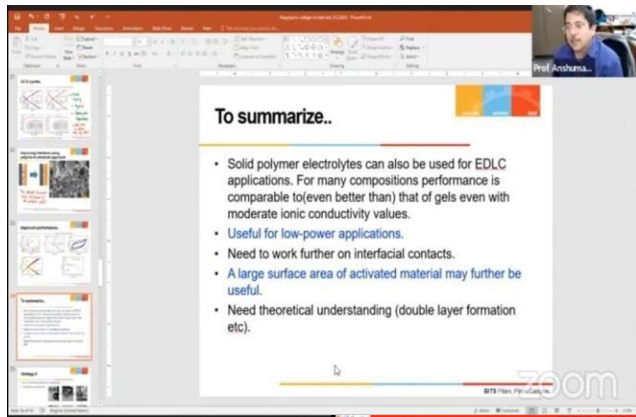
**Technical Session-2 (11:00 am-1:30 pm) -**

On Second day of the The workshop IWESSM 2023 in the second technical session there werethree invited talks Namely by Prof.Anshuman Dalvi, Dr. R. K. Gupta and Dr. Mohan L. Verma.

The program Started with a Talk by Prof. Anshuman Dalvi from BITS Pilani Campus Rajasthan. He elaborated on the subject of Solid State super capacitor's fundamental fabrication strategies and challenges. Ms. Manisha Gupta of Department of Physics gave Vote of thanks to Prof. Dalvi.

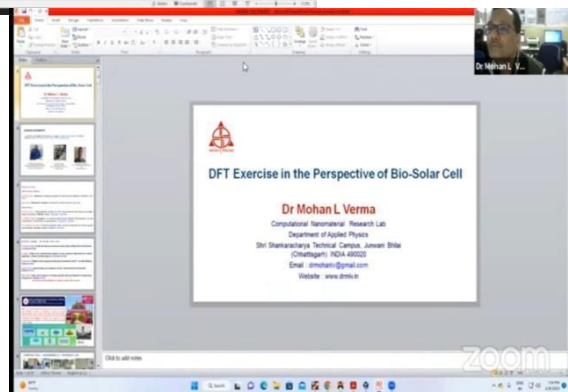
Then second invited talk was taken on the topic Solar Cells and how silicon based Solar Cells are important in Energy Generation by DR. Ravindra. K. Gupta who joined us in Online mode from Saudi Arabia. He also explained about various materials used in manufacturing of Solar Cell and compared different Results usingGraphs. Ms. Rashmi Priya Toppo of Department of Physics gave Vote of thanks to Prof. Gupta.

In third invited talk Prof. Mohan L Verma from SSTC, Bhilai gave his Insights on DF Theory. He showed different Research paper to students and talk about Simulation process in Detail.Prof. Vinod Kumar Dubey of Department of Physics gave Vote of thanks to Prof. Verma.



## Contents

- Sunlight
- Solar Cells (SCs)
- Silicon-based SCs
- III-V Elements-based SCs
- Chalcogenide-based SCs
- Quantum-dot-Sensitized SCs
- Organic SCs
- Perovskite SCs
- Dye-Sensitized Solar Cells
- Confirmed Solar Cell Efficiencies of Terrestrial Modules
- Collaborators
- Acknowledgements



### Hands on Session -2 (2:30 pm -4:30 pm)-

A Hands on Session in second half of the program was taken by Dr. Mohan L Verma SSTC, Bhilai and Dr Narendra Bansal of Abu Dhabi. The optimization process of material simulation was explained in detail and gave the brief idea about DoS (density of state) of material under study.



### Day-3, 10.02.2023

### Technical Session-3 (11:00 am-1:30 pm) -

On Third and last day of the workshop IWESSM 2023

the program started with a talk by Dr. Pritam Kumar Panda from Uppsala University of Sweden. He talked about Genome to Quinome: Translational paradigm interfacing molecule with nano materials. Ms Rashmi Priya Toppo gave vote of thanks to Dr. Panda for his insight.

On Second invited talk was taken on the topic synthesis and

characterization of multi-component alloys by Dr. Manwendra Tripathi of NIT Raipur. Ms Manisha Gupta gave vote of thanks to Dr. Tripathi after his discussion.

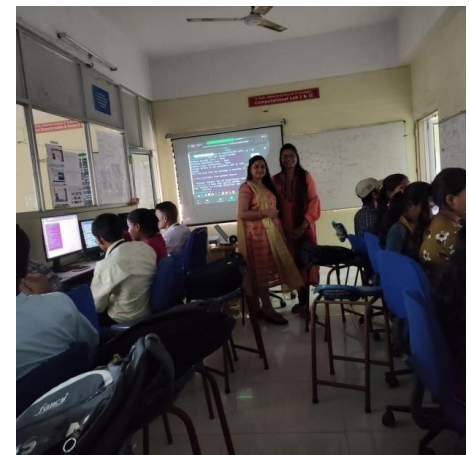
In Next part of the program HoD of Physics Department GNSC and Chairperson Dr Anjali Oudhia gave a talk on study of electronic and optical properties by SIESTA. Ms Rashmi Priya Toppo gave vote of thanks to Prof. Anjali Oudhia for her discourse.



### Hands on Session -3 (2:30 pm -4:30 pm)

In second half of the program practical session was taken by Dr. Mohan L Verma SSTC, Bilai and Dr Narendra Kumar of Abu Dhabi. In this session the PDoS (projected density of state), charge density, band gap, optical properties and the plotting of their graphs were discussed in detail.

With this Final session the 3 days International Workshop ended successfully and Students gave their valuable remarks.



### Valedictory function (Day-3, 4:30pm-4:45pm)

In the valedictory session Dr. Alok Luka Organizing Secretary of the seminar presented the report of the three days international workshop. Prof. Anjali Oudhia, HOD Physics Govt. Nagarjuna PG College of Science, Raipur in her address applauded the members of organizing committee for organizing this joint venture and also appreciated CGCOST for their support. In the end Prof Oudhia gave vote of thank to all who participated and gave their valuable insight on the subject.



**You Tube Links:**

**Official channel link:** <https://youtube.com/@physicsDepartment.gnsraipur>

**Facebook link:**

[https://www.facebook.com/profile.php?id=100088683115426&mibextid=ZbWKw\\_L](https://www.facebook.com/profile.php?id=100088683115426&mibextid=ZbWKw_L)

**Inaugural function:** <https://www.youtube.com/live/KcViFcEkCWs?feature=share>

**TechnicalSession day-1**

[https://www.youtube.com/live/ja0\\_BYWDCaA?feature=share](https://www.youtube.com/live/ja0_BYWDCaA?feature=share)

**TechnicalSession day-2**

<https://www.youtube.com/live/8oIlhHeELBg?feature=share>

**TechnicalSession day-3**

<https://www.youtube.com/live/3GJIaKJI6gA?feature=share>

**Hands on session day -1** <https://youtu.be/yLqqbHJLJLk>

**Hands on session day- 2** <https://youtu.be/nyGXLhrtnew>

**Hands on session day -3** [https://youtu.be/VtvZT\\_2q58s](https://youtu.be/VtvZT_2q58s)