



(NSCM -2024)

**National Symposia on Innovation in Computational Methods**

**October 22-23, 2024**

**SoS in Physics & Astrophysics**

**Pt. Ravishankar Shukla University, Raipur, 492010, (C.G) INDIA**

## Technical Report

National Symposia on Innovation in Computational Methods was organized by School of Studies in Physics and Astrophysics, Pt. Ravishankar Shukla University, Raipur. It was two days National symposia held during October 22-23, 2024.

The Inauguration session of the symposia was held on 22.10.2024. Prof. A. C. Pandey, Director IUAC New Delhi (chief guest), senior professors Prof. S. K. Pandey Former Vice Chancellor of Pt. RSU, Prof. Y. M. Gupta and Prof. Ravindra Pandey, Michigan Tech University, Michigan, USA were guest of honour of this conference. After the formal inauguration, Dr. Y. K. Mahipal, convener of the symposia gave the welcome Address and brief introduction about the symposia and Prof. Nameeta Brahme introduce the department and their achievements.



### **Technical Session I**

The first technical session of the symposia has started with the talk of Prof. A. C. Pandey. He started his talk with the history of physics and its connection with mathematics and later on its connection with simulation. Furthermore, the speaker explained the prediction of weather forecast as well designing of MRI machines on the basis of Simulation in a very simple way.

Second technical talk of this session was delivered by Prof. Sandeep Nigam, Chemistry Division, BARC Mumbai. The topic of his talk is “Discerning the link of computational methods on experiments: connecting few dots”. The talk started with connecting experimental observation with

theoretical models proposed by computational methods. Initially the speaker deals with some basic terminology of Quantum and classical mechanics then comes to the Density Functional Theory. Prof. Sandeep beautifully explains the expectations of theoretical models and the originality. Later on, he focused on how to come know about the exact problem and their resolution in enhancing the luminescent properties of nanophosphors via computational methods with the example of  $Y_2Ge_2O_7:Eu$ .



## Technical Session II

In this session, Invited talks were delivered by Prof. Prof. Ravindra Pandey from Michigan Tech University, Michigan. His talk is based on the modelling of 2D material using first principle DFT theory. He started his talk with brief introduction about simulation methods, range of materials for simulation, characterization techniques and synthesis. He further explains how a band gap is created in a zero band gap material by considering the concept of heterostructure. He also manifest the verification of modelled materials experimentally through some examples.



## Second Day 22.10.2024

### Technical Session III

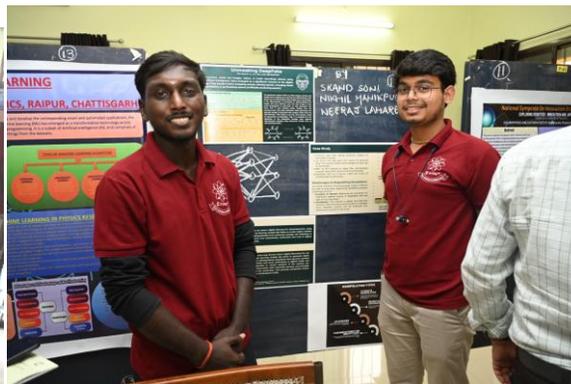
On 23.10.2024, the technical session was start with the talk of Prof. Naresh K Nagwani, Dept of Computer Science & Engineering, NIT Raipur. He explained the quantum computing with the help of Gaussian software. After that Prof. M. N. Tripathi, Guru Ghasidas (Central) University, Bilaspur was delivered his talk on the topic of "Density Functional Theory (DFT)". The speaker introduce about DFT and tell that how to find the ground state energy of any molecule using DFT.

There after he also provides the hands on training to the research scholars by using Gaussian Software. In the parallel session Prof. Sandeep Nigam interact with M. Sc. Students.

### Technical Session IV

In this session Dr. Laxmi Kant, delivered talk in the topic of "Accelerating Physics with Python: An Introduction". He highlighted Python's significance in modern physics, emphasizing particularly in visualizing data and conceptual frameworks, effectively bridging theoretical insights with practical applications.

In this symposium more than 100 students are participated. 40 posters were displayed by the participants.



On Valedictory function, Convener of the conference Dr. Y. K. Mahipal has delivered brief report of the conference. The Prof. Y. M. Gupta (Chief guest), Prof. R. N. Baghel (Special Guest) were present in this function.

In this function the best two poster presentations have awarded with cash price. Mr. Chitrkant Belodiya gave vote of thanks on behalf of organizing committee.



**Convener**

**Dr. Y. K. mahipal**