UNIVERSITY GRANTS COMMISSION (UGC)

MALVIYA MISSION TEACHER TRAINING CENTRE

TECHNICAL REPORT

Refresher Course
In
Computational Sciences

(Chemistry, Physics, Computer Science, Electronics, Mathematics and Statistics)

September 9 – 23, 2024

Pt. Ravishankar Shukla University, Raipur (C.G.)

Organizing Team

Prof. Sachchidanand Shukla
Vice Chancellor
Pt. Ravishankar Shukla University,
Raipur

Prof. Preeti Suresh
Director, HRDC
Pt. Ravishankar Shukla University, Raipur

Dr. Kallol K. Ghosh
Course Coordinator, S.O.S.
in Chemistry,Pt. RSU, Raipur

Dr. Arvind Agrawal
Course Coordinator HRDC,Pt. RSU,
Raipur (C.G.)

List of Participants

S. No.	Name of the Participants	College/Institute Address	Affiliated University	Mobile No.	Email Address
1.	Mr. Chitrkant Belodhiya	SoS in Physics and Astrophysics Pt. Ravishankar Shukla University, Raipur (C.G.)	Pt. Ravishankar Shukla University, Raipur (C.G.)	7587253783	ckbelodhiya@gmail.com
2.	Shail Kumari Sharma	Govt. Pt. J. L. N. Arts and Science P. G. College, Bemetara(C.G.)	Hemchand Yadav University, Durg (C.G.)	7974516354	shailsharma2705@gmail. com
3.	Dr. Swati Jain	Government J. Yoganandam Chhattisgarh College, Raipur (C.G.)	Pt. Ravishankar Shukla University, Raipur (C.G.)	9407677567	sjcscghed@gmail.com
4.	Dr. Bhupendra Kumar Sen	Govt. College, Ramchandrapur	Sant Gahira Guru University, Ambikapur (C.G.)	9098710075	senbk20@yahoo.in
5.	Mr. Dildar Singh Tandon	Govt. Agrasen College Bilha, Dist. - Bilaspur, Chhattisgarh	Atal Bihari Vajpayee University, Bilaspur (C.G.)	9827462154	dildartandon1983@gmail. com
6.	Mr. Shashank Singh Rathore	Veerangna Rani Durgawati Govt Girls College, Takhatpur	Atal Bihari Vajpayee University, Bilaspur (C.G.)	7354923619	shashankorgchem@gmail.com
7.	Dr. Yugal Kishor Mahipal	School of Studies in Physics and Astrophysics Pt. Ravishankar Shukla University, Raipur (C.G.)	Pt. Ravishankar Shukla University, Raipur (C.G.)	7999970312	ykmahipal@gmail.com
8.	Dr. Indrapal Karbhal	School of Studies in Chemistry Pt. Ravishankar Shukla University, Raipur (C.G.)	Pt. Ravishankar Shukla University, Raipur (C.G.)	8605985169	ikarbhal@gmail.com
9.	Mr. Lokesh Kumar Satpathi	Government Naveen College Gudhiyari, Raipur, (C.G.)	Pt. Ravishankar Shukla University, Raipur (C.G.)	8319736662	lokeshsatpathi@gmail.co m
10.	Dr. Govind Prasad Sahu	Center for Basic Sciences, Pt. Ravishankar Shukla University, Raipur (C.G.)	Pt. Ravishankar Shukla University, Raipur (C.G.)	9926963899	govind3012@gmail.com

11.	Dr. Bhanushree Gupta	Center for Basic Sciences, Pt. Ravishankar Shukla University, Raipur (C.G.)	Pt. Ravishankar Shukla University, Raipur (C.G.)	7974626126	bgupta1517@gmail.com
12.	Mrs. Vaishnavi Mandavi	Govt. Danteshwari P.G. Girls College, Jagdalpur (C.G.)	Shaheed Mahendra Karma Vishwavidyalaya, Bastar, Jagdalpur, Dist.-Bastar, (C.G.)	7470542607	vaishnani.markam@gmail.com
13.	Dr. Deena Sunil	Indira Gandhi National Tribal University, Amarkantak (M.P.)	Indira Gandhi National Tribal University, Amarkantak (M.P.)	7090070004	deenasunil00007@gmail. com
14.	Megha Sahu	S. o. S. in Electronics, Pt. Ravishankar Shukla University Raipur	Pt. Ravishankar Shukla University, Raipur (C.G.)	6263881395	mgsahu1610@gmail.com
15.	Tripti Verma				
16.	Dr. Shradhha Shukla	Center for Basic Sciences, Pt. Ravishankar Shukla University, Raipur (C.G.)	Pt. Ravishankar Shukla University, Raipur (C.G.)	799915389	
17.	Dr. Vandana Singh	S. o. S. in Chemistry Pt. Ravishankar Shukla University Raipur	Pt. Ravishankar Shukla University, Raipur (C.G.)	8349764681	Vanda.gpa@gmail.com
18.	Dr. Bhunewswari Sahu	S. o. S. in Chemistry Pt. Ravishankar Shukla University Raipur	Pt. Ravishankar Shukla University, Raipur (C.G.)	7898754055	bhunewari90@gmail.com
19.	Dr Deepti Pateria	Pt. Ravishankar Shukla University, Raipur (C.G.)	Pt. Ravishankar Shukla University, Raipur (C.G.)	9993489867	deepti_rpr@rediffmail.co m

UGC - MMTTC, PRSU, Raipur

Final Time Table: Refresher Course in Computational Science (09.09.2024 to 23.09.2024)

Refresher Course in Computational Science **(09.09.2024 to 23.09.2024) UGC-MMTTC** **Pt. Ravishankar Shukla University, Raipur 492 010, Chhattisgarh**				
Day/ Date	**Session -I (10:30 to 12:00**	**Session -II (12:15 to 13:45)**	**Session -III (14:15 to 15:45)**	**Session –IV (16:00 to 17:30)**
Day 01 (09.09.24)	**Registration Inauguration Induction**	**Lecture-1** **Prof. Mohan Lal Verma** *SSTC, Bhilai* **Frontiers & Challenges of Computational Sciences**	**Lecture-2** **Dr. Sharada Nandan Raw** *NIT Raipur.* **Fundamentals of Mathematical Modeling in Real World and Trends in Mathematics on Social Media**	**Lecture-3** **Prof. Mohan Lal Verma** *SSTC, Bhilai* **A Hands on Training on How to use DFT Tools**
Day 02 (10.09.24)	**Lecture-4** **Prof. Mohan Lal Verm** *SSTC, Bhilai* **Opto Elecronics & Electrochemical Device Modeling with DFT**	**Lecture-5** **Dr. Sharada Nandan Raw** *NIT Raipur.* **An Appease Introduction of Theoretical Aspects and Concepts on Dynamical System and Chaos**	**Lecture-6** **Dr. Santosh Singh Thakur** *GGU Bilaspur* **Application of Density Functional Theory for the Calculation of Infrared and Vibrational Circular Dichroism Spectra of Valuable Chiral Molecules**	**Lecture-7** **Prof. B. Keshav Rao** *SSTC, Bhilai* **2D-Hybrid/Polymer Materials - A DFT Study**
Day 03 (11.09.24)	**Lecture-8** **Prof. B. Keshav Rao** *SSTC, Bhilai* **Gas Sensing Device based on Defective Graphene**	**Lecture-9** **Prof. Naresh Kumar Nagwani** *NIT Raipur* **An Overview of Data Visualization Techniques (with an overview of Python and R Libraries)**	**Lecture-10** **Prof. Sanjay Kumar** *School of Studies in Computer Science & IT PRSU Raipur* **High-Performance Computer Part-1**	**Micro Teaching Prof. Kamlesh K. Shrivas** *PRSU Raipur* **S.No: 1-7**
Day 04 (12.09.24)	**Lecture-11** **Prof. Naresh Kumar Nagwani** *NIT Raipur* **Applications of Machne Learning in Various Domain.**	**Lecture-12** **Prof. Sudipta Kanungo** *IIT GOA* **Density Functional Theory-I: Concept and Methodology.**	**Micro Teaching** **Prof. Kamlesh K. Shrivas** *PRSU Raipur* **S.No: 8-14**	**Micro Teaching** **Prof. Kamlesh K. Shrivas** *PRSU Raipur* **S.No: 15-20**

(Column separators: Lunch Break, Tea Break)

Day					
Day 05 (13.09.24)	**Lecture-13** **Prof. Sudipta Kanungo** *IIT Goa* **Beyond Standard DFT: Spin and Correlation**	**Lecture-14** **Prof. Khemchand Dewangan** *GGU, Bilaspur* **Learning Chemistry Through Computers**	**Lecture- 15** **Prof K. Srinivas** *NIEPA , New Delhi.* **NEP 2020: ICT Skills and competencies for Interactive and Personalised Learning**	**Lecture-16** **Prof K. Srinivas** *NIEPA , New Delhi.* **Designing and Developing Interactive Video Content for effective Teaching & Learning**
Day 06 (14.09.24)	**Lecture-17** **Prof K. Srinivas** *NIEPA , New Delhi.* **Open Educational Resources and Transformative** **Teaching- Learning Practices**	**Lecture-18** **Prof K. Srinivas** *NIEPA , New Delhi.* **Exploring** **Learning Management Systems for enhanced Learning Experiences.**	**Lecture-19** **Prof. Madhvendra Nath Tripathi** *GGU, Bilaspur* **Quantum Mechanical Modelling Methods: Genesis and applications**	**Lecture-20** **Prof. Khemchand Dewangan** *GGU, Bilaspur* **Fundamentals and Applications of Density Functional Theory**
Day 07 (16.09.24)	**Lecture-21** **Prof. Madhvendra Nath Tripathi** *GGU, Bilaspur* **Designing the Materials for Desired Properties by Density Functional Theory**	**Tea Break** / **Lecture-22** **Prof. Madhvendra Nath Tripathi** *GGU, Bilaspur* **Hands on Training on DFT**	**Lunch Break** / **Lecture-23** **Prof. Sanjay Kumar** *School of Studies in Computer Science & IT PRSU Raipur* **High-Performance Computer Part-1**	**Tea Break** / **Lecture-24** **Prof. O P VYAS** *IIIT ALLHABAD* **Foundations of Process Science: Process Modelling.**
Day 08 (18.09.24)	**Lecture-25** **Prof. Kamlesh Shrivas Pt. R S Univ Role of Statistics in Computational Sciences and Scientific Research**	**Seminar** **Prof. Manas Kanti Deb** *PRSU Raipur* **S.No: 1-6**	**Lunch Break** / **Seminar** **Prof. Manas Kanti Deb** *PRSU Raipur* **S.No: 7-12**	**Lecture 26** **Dr. Vinod Kumar Patle** **SoS in Computer Sci . PRSU** "The New Paradigm of Information Technology."

Day 09 **(19.09.24)**	**Lecture 27** **Dr. Md Mehboob Alam** *IIT Bhilai* **Basic quantum to computational methods**	**Lecture-28** **Dr. Md Mehboob Alam** *IIT Bhilai* **Simulating Geometry and some spectroscopic properties**	**Seminar** **Prof. Manas Kanti Deb** *PRSU Raipur* **S.No: 13-20**	**Lecture 29** **Prof. Balwant Singh Thakur** *SoS in Mathematics,PRSU* "**Evaluating Research Impact in Computational Sciences: Understanding Journal Impact Factor & Author Matrices .**"
Day 10 **(20.09.24)**	**Lecture-30** **Dr. Vinod Kumar Patle** SoS in Computer Sci . PRSU "Learning Management System with Moodle"	**Lecture-31** **Research Project Preparation** **&** **Visit to Computer Lab, NCNR, CBS**	**PROJECT** **Dr. Gourisankar Roymahapatra** *HIT, HALDIA* **S.No: 1-10**	**PROJECT** **Dr. Gourisankar Roymahapatra** *HIT, HALDIA* **S.No: 11-20**
Day 11 **(21.09.24**	**Lecture-30** **Dr. Md Mehboob Alam** *IIT Bhilai* **Basics of molecular dynamics and genetic algorithm**	**Lecture-31** **Dr. Md Mehboob Alam** *IIT Bhilai* **Hands-on molecular dynamics simulation**	**Lecture-32** **Prof. S. R. Gadre** *Savitribai Phule Pune Univ., Pune* **Storage of Numbers in a Computer, Roundoff Errors,** **Trunation Error**	**TEST**
Day 12 **(23.09.24)**	**Lecture 33** **Prof. S. R. Gadre** *Savitribai Phule Pune Univ., Pune* **Our Story of Indigenous Quantum Chemistry Algorithm and Code Development**	**VALEDICTORY**		

Report-Day-1 (09/09/2024)
Refresher Course in Computational Science
UGC-MMTTC, Pt. Ravishankar Shukla University – Raipur (C.G.)
Chairman/Reporter: Dr. Indrapal Karbhal

The **Refresher Course in Computational Science** at **UGC-MMTTC, Pt. Ravishankar Shukla University, Raipur (C.G.) (09-23 September 2024)** commenced on 09 September 2024 at **10:30 AM**. The program was inaugurated by the **Honorable Vice-Chancellor, Prof. Sachchidanand Shukla**. **Prof. Kallol K. Ghosh**, the **Course Coordinator**, facilitated a concise introductory session, providing an overview of the experts and their respective lecture topics.

Prof. Preeti K. Suresh, Director of MMTTC, highlighted the significance of both the online and offline components of the course, emphasizing the unique benefits of the offline format, such as direct interaction with subject matter experts and peer participants.

The **Honorable Vice-Chancellor, Prof. S. N. Shukla**, also addressed the pivotal role of computational science and theoretical calculations in fostering multidisciplinary education. He underscored its future relevance across various fields such as medicine, mathematics, physics, chemistry, electronics, space engineering, botany, and zoology, envisioning how such research initiatives will spark innovation and creative thinking among the younger generation.

The participants introduced themselves briefly, and the inaugural session concluded with a vote of thanks delivered by Dr. Arvind Agrawal.

Session-II (12:15 to 13:45 pm), commenced with a lecture by **Prof. Mohan L. Verma,** Professor and Head of the Department of Applied Physics, and Dean of Applied Science at CSVTU, Shri Shankaracharya Technical Campus, Bhilai (SSTC). The session, titled ***"Frontiers & Challenges of Computational Sciences"*** was highly interactive and insightful.

Prof. Verma delivered an engaging talk on the challenges and frontiers in computational sciences, elaborating on molecular modeling, Density Functional Theory (DFT), and electronic structure theory (EST). He also demonstrated the use of the

SIESTA program tools for calculating electronic structural parameters such as HOMO-LUMO levels and other energy-related parameters, explaining their applications in chemistry, physics, and mathematics. Notably, he highlighted that SIESTA is open-source software, accessible for both students and teachers for educational and research purposes, emphasizing the significance of such tools in predicting experimental outcomes in the near future. The session concluded with an engaging question-and-answer round.

Session-III (02:15 to 03:45 pm), was led by **Dr. Sharad Nandan Raw,** Associate Professor at the Department of Mathematics, National Institute of Technology (NIT) Raipur (CG). His talk, titled ***"Fundamentals of Mathematical Modeling in the Real World and Trends in Mathematics on Social Media"*** focused on the foundational concepts of mathematical modeling.

Dr. Raw discussed how mathematical modeling is applied to solve real-world problems, highlighting current trends in the field, especially as seen on social media platforms. He provided insights into the essential steps involved in constructing mathematical models for real-world issues, and concluded with a discussion on the significance of mathematical modeling and its wide-ranging applications.

Session-IV (16:00 to 17:30 pm) was once again led by **Prof. Mohan L. Verma**, who conducted a hands-on training session titled ***"A Hands-on Training on How to Use DFT Tools"*.** In this session, Prof. Verma explained the basic system requirements for running DFT tools and introduced key software tools, which he categorized into three groups: (i) pre- processing tools, such as material design software, (ii) main DFT tools, used to optimize materials of various shapes and sizes, and (iii) post-processing tools, including visualization and plotting programs. Participants were given the opportunity to perform hands-on exercises with molecules and nanotubes, applying the techniques discussed during the session.

Glimpses of the Day 1 (9ᵗʰ September 2024)

3

Report-Day-2 (10/09/2024)
Refresher Course in Computational Science
UGC-MMTTC, Pt. Ravishankar Shukla University – Raipur (C.G.)
Chairman/Rapporteur: Chitrkant Belodhiya

Session- I (10:30 am to 12:00 Noon), The session, titled **"Opto Electronics & Electrochemical Device Modeling with DFT"** was highly interactive and insightful. It commenced with a lecture by **Prof. Mohan L. Verma,** who is the Professor and Head of the Department of Applied Physics and the Dean of Applied Science at CSVTU, Shri Shankaracharya Technical Campus, Bhilai (SSTC).

Dr. M.L. Verma lecture delved into the application of novel materials in various optoelectronic and electrochemical devices, focusing on the modeling of these devices using Density Functional Theory (DFT). The lecture covered the evolution of device types, the nature of materials used, and the challenges faced in device modeling. A comparative overview of different supporting tools for characterizing these devices was also provided. The session wrapped up with a dynamic and interactive Q&A segment.

Session-II (12:15 to 13:45), The session was led by **Dr. Sharad Nandan Raw**, an Associate Professor in the Department of Mathematics at the National Institute of Technology (NIT) Raipur (CG). His talk, titled **"An Appeasing Introduction to Theoretical Aspects and Concepts on Dynamical Systems and Chaos,"** focused on the foundational concepts of mathematical modeling.

Dr. Sharda Nandan Raw lecture offered a comprehensive introduction to the theoretical aspects of dynamical systems and chaos. The discussion covered fundamental concepts, highlighted the beauty of chaotic systems, and introduced key tools for detecting and analyzing chaos. The

use of examples provided practical insights into the application of these concepts, enhancing the audience's understanding of dynamical systems and chaos theory.

Session-III (14:15 to 15:45) The session was led by **Dr. Santosh Singh Thakur**, an Associate Professor in the Department of Chemistry at Guru Ghasidas Vishwavidyalaya (GGU), Bilaspur (C.G.). His talk, titled *"Application of Density Functional Theory for the Calculation of Infrared and Vibrational Circular Dichroism Spectra of Valuable Chiral Molecules,"* focused on the versatility of Density Functional Theory (DFT) in computational chemistry and its significance in analyzing and interpreting spectroscopic data.

Dr. Santosh Singh Thakur lecture provided a comprehensive overview of the application of DFT in calculating IR and VCD spectra for chiral molecules. The talk demonstrated the power of DFT in computational chemistry and its role in analyzing molecular properties and stereochemistry. The use of the B3LYP hybrid functional and Gaussian program for these calculations highlights the advancements in computational methods and their practical applications in research and industry.

Session-IV (16:00 to 17:50) The session was led by **Dr. B. Keshav Rao**, an Associate Professor of Applied Physics at Shri Shankaracharya Technical Campus, Bhilai (C.G.). His talk, titled *"2D-Hybrid/Polymer Materials - A DFT Study"* focused on a first-principles study using Density Functional Theory (DFT) to investigate the effects of doping and external factors on the properties of 2D hybrids and 3D polymer hybrids.

Dr. B. Keshav Rao lecture provided a comprehensive overview of the DFT-based study of 2D hybrid materials and 3D polymer hybrids, highlighting the effects of doping, strain, electric fields, and molecular dispersion on their properties. The findings underscored the importance of understanding and controlling these factors to optimize the materials' electronic and mechanical behavior for advanced technological applications. The study's insights into band-gap modulation, stability, and material transformation have significant implications for the development of next-generation electronic and optoelectronic devices.

Glimpses of the Day 2 (10ᵗʰ September 2024)
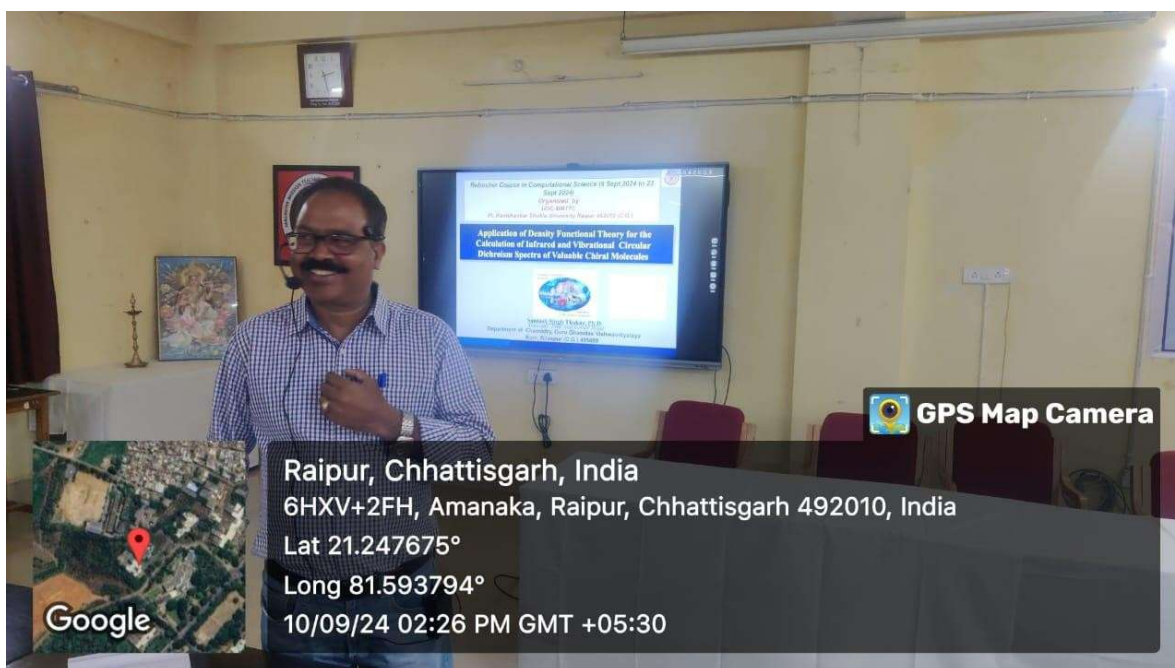
Report-Day-3 (11/09/2024)
Refresher Course in Computational Science
UGC-MMTTC, Pt. Ravishankar Shukla University – Raipur (C.G.)
Chairman/Reporter: Dr. Govind Prasad Sahu

The first session of the third day of the refresher course started at 10.30 am on 11-09-2024. **Dr. B. Keshav Rao**, associate professor, Shri Shankaracharya Technical Campus, Junwani, Bhilai, Chhattisgarh, delivered an insightful lecture on the use of defective graphene for gas sensing devices. His research on this topic is of significant importance, as he elaborated on how defects in graphene's structure can significantly alter its electronic properties, making it highly effective for detecting various gases such as CO, CO2, and NH3. Dr Rao's work in this area is particularly crucial as it opens up new possibilities for gas-sensing technologies. He described the types of defects that can occur in graphene, including pentagonal, heptagonal, and octagonal defects, each contributing to different changes in graphene's electronic behaviour. He emphasized the importance of line defects and their role in enhancing the sensitivity of graphene-based gas sensors.

Dr. Rao's lecture not only provided a comprehensive overview of the interplay between graphene's structural defects and its functional applications in sensing technologies but also highlighted the broader potential of graphene. He noted its potential in various fields beyond gas sensing due to its unique properties that can be tailored through defect engineering. This broader perspective enhances the audience's understanding of graphene's versatility and its potential impact in diverse fields.

The second session started at 12:00 pm. Resource person **Prof. Naresh Kumar Nagwani**, the Head of the Department of Computer Science and Engineering (CSE) at the National Institute of Technology (NIT), Raipur, delivered an insightful lecture on "An Overview of Data Visualization Techniques." His talk focused on explaining the concept and importance of data visualization in modern data analysis. Prof. Nagwani emphasized that data visualization is a powerful tool that enables the clear and effective presentation of complex data, making

patterns, trends, and outliers more comprehensible to users. He highlighted that visual representations not only help to bridge the gap between data analysis and decision-making but also empower the audience by enhancing the communication of information. Furthermore, he introduced the audience to different types of data visualization techniques, ranging from simple charts and graphs to more advanced visualizations like heatmaps and geographic maps.

In addition to the theoretical aspects, Prof. Nagwani also discussed practical tools available for data visualization, such as Python and R libraries, which are widely used in data science. He gave a brief overview of how datasets can be processed and visualized using these libraries, demonstrating the ease with which different types of data can be represented. He also introduced the concept of a "word tree," which is a visual tool for text data, helping to uncover the relationships and frequencies of words in large textual datasets. The lecture concluded with practical insights into how effective visualizations can enhance data interpretation, especially in research and business decision-making processes.

In the third session (2:15 to 3:45 PM), **Prof. Sanjay Kumar**, the Head of the School of Studies in Computer Science and IT, Pt. Ravishankar Shukla University, Raipur, delivered a lecture on "High Performance Computing" (HPC). He began by tracing the history of computation, highlighting the evolution from early mechanical devices to modern digital computers. Prof. Kumar explained how computational demands have increased exponentially over time, leading to the need for more powerful computing systems. He stressed that traditional computing approaches were no longer sufficient to handle large-scale, complex problems, which is where high-performance computing comes in. By utilising multiple processors simultaneously, HPC accelerates computational processes, making it possible to solve problems that would otherwise take too long on conventional systems.

Prof. Kumar also discussed the key concepts of parallel computing and distributed computing, which are fundamental to HPC. He explained parallel computing as the simultaneous execution of multiple tasks to break down large problems into smaller parts, allowing faster processing. Similarly, distributed computing, where tasks are distributed across multiple machines or systems, enables efficient handling of enormous datasets and complex calculations. Throughout the lecture, Prof. Kumar explained these technical concepts in a

simple, approachable manner, ensuring that participants from various backgrounds could understand the importance and application of high-performance computing in modern scientific research, engineering, and business domains.

The fourth and last session of the day started at 4:00 p.m. with micro-teaching by the participants. **Prof. Kamlesh Shrivas**, a professor at the School of Chemistry Studies, Pt. Ravi Shankar Shukla University, Raipur, examined the micro-teaching. At the end, he explained the participants' critical performance in the micro-teaching and gave suggestions for improvements.

The session ended with a vote of thanks by Dr. Govind Prasad Sahu (Chairman)

Glimpses of the Day 3 (11th September 2024)

9
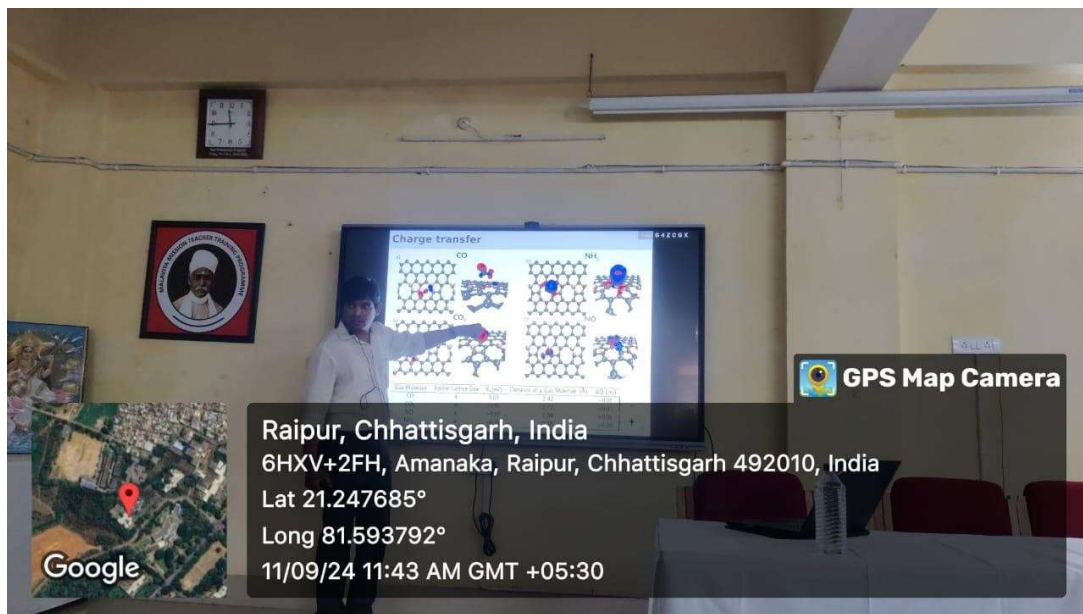
Report-Day-4 (12/09/2024)
Refresher Course in Computational Science
UGC-MMTTC, Pt. Ravishankar Shukla University – Raipur (C.G.)
Chairman/Reporter: Dildar Singh Tandon

The first session of the fourth day of the refresher course began at 10:30 AM on September 12, 2024. The session featured an insightful lecture by **Prof. Naresh Kumar Nagwani**, Head of the Department of Computer Science and Engineering (CSE) at the National Institute of Technology (NIT), Raipur. Prof. Nagwani delivered a comprehensive talk on *"Applications of Machine Learning in Various Domains."* He discussed common and popular machine learning technologies, such as classification, clustering, regression analysis, and association rule mining, along with examples and their applications.

Prof. Nagwani highlighted how Machine Learning (ML) has become a transformative technology across various fields, revolutionizing industries by enabling systems to learn from data and make predictions or decisions without explicit programming. He elaborated on the diverse applications of ML, explaining how it is used in healthcare for diagnosing diseases, predicting patient outcomes, and personalizing treatment plans. In finance, ML is employed for fraud detection, algorithmic trading, and credit scoring. In the realms of e-commerce and marketing, ML powers recommendation systems, customer segmentation, and demand forecasting. He also discussed the role of ML in autonomous vehicles, which rely on real-time decision-making and navigation.

Furthermore, Prof. Nagwani explained the use of ML in natural language processing (NLP) for language translation, sentiment analysis, and virtual assistants. He concluded by highlighting how industries like manufacturing, energy, and cybersecurity benefit from ML by optimizing operations, predicting maintenance needs, and enhancing threat detection. Prof. Nagwani's lecture provided a thorough understanding of the widespread impact and potential of machine learning across various domains.

10

The second session began at 12:15 PM, featuring a lecture by **Dr. Sudipta Kanungo**, an Associate Professor at the School of Physical Sciences, Indian Institute of Technology (IIT) Goa. Dr. Kanungo's lecture was focused on ***"Density Functional Theory: Concepts and Methodology."*** He started by introducing the basic concepts and methodology of density functional theory (DFT). He briefly covered the many-electron problem using the Hamiltonian, transitioning from general wave function methods like Hartree and Hartree-Fock to the density functional-based approach.Dr. Kanungo discussed key theorems such as the Hohenberg-Kohn and Kohn-Sham theorems, including their derivations. He also introduced the concepts of basis sets and pseudopotentials, explaining their importance in the current context. In the latter part of the lecture, he covered exchange-correlation functionals and relevant approximations, highlighting the successes and limitations of DFT in calculating various properties. Dr. Kanungo's presentation provided a comprehensive overview of DFT, bridging foundational concepts with practical applications.

The third and fourth sessions of the day commenced at 2:15 PM, featuring micro-teaching presentations by the following participants: Dr. Indrapal Karbhal, Mr. Lokesh Satpat, Dr. Govind Prasad Sahu, Dr. Bhanushree Gupta, Dr. Deena Soni, Dr. Vaishanavi, Dr. Swati Jain, and Dr. Deepti Pateria. The micro-teaching sessions were evaluated by **Prof. Kamlesh Shrivas**, a professor at the School of Chemistry Studies, Pt. Ravi Shankar Shukla University, Raipur. At the end of the sessions, Prof. Shrivas provided feedback on the participants' performances, highlighting areas for improvement and offering constructive suggestions.

The session concluded with a vote of thanks delivered by Dildar Singh Tandon, the Chairman.

Glimpses of the Day 4 (12ᵗʰ September 2024)
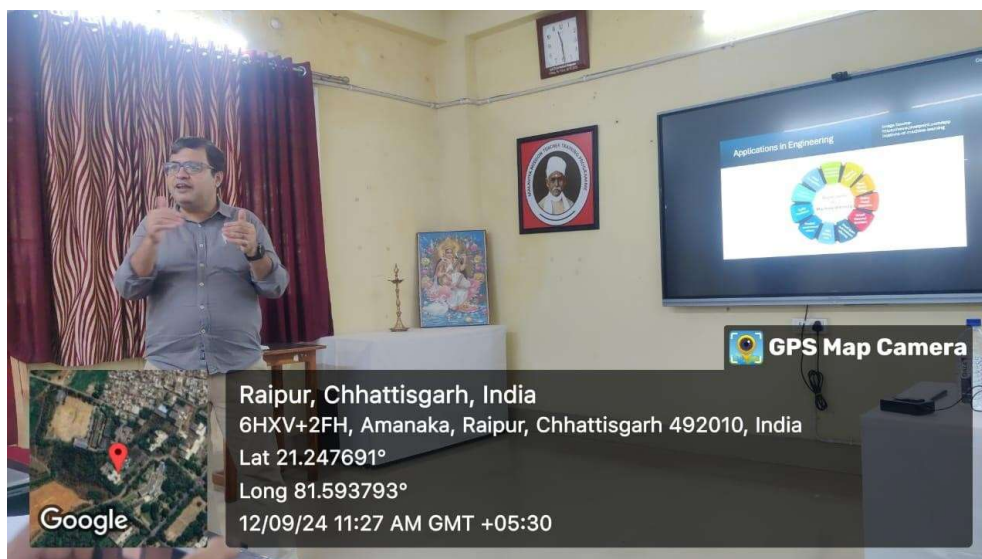
Report-Day-5 (13/09/2024)
Refresher Course in Computational Science
UGC-MMTTC, Pt. Ravishankar Shukla University – Raipur (C.G.)
Chairman/Reporter: Dr. Y. K. Mahipal

First Session of the 5th day of Refresher Course started at 10: 30 am. **Dr. Sudipta Kanungo** is an Associate Professor in School of Physical Sciences, Indian Institute of Technology (IIT), Goa. He has delivered a lecture *entitled "Beyond Standard Density Functional Theory (DFT): Spin and Correlation"*. Dr. Kanungo has focused the role of DFT on strong electron – electron interaction and their importance on magnetism. He has also explained the effect of the electron motion in the solid can be addressed via DFT framework.

Second Session is started at 12: 15 o'clock. **Prof. Khemchand Dewangan** is presently working as a Professor of Chemistry in Department of Chemistry, Guru Ghasidas (Central) University, Bilaspur (CG). He has delivered a lecture entitled *"Learning Chemistry Through Computers"*. Prof. Dewangan has focused on the role of Computer software to learn Chemistry and the applications of educational software, online courses and tutorials including virtual labs.

Third session is started at 2.15 pm. Prof. K Srinivas is presently working a Head, ICT & Project management Unit and Chairperson e-learning cell, National Institute of Educational Planning and Administration (NIEPA), New Delhi.

Prof. K Srinivas has delivered a lecture entitled *"NEP – 2020: ICT Skills and Competencies for Interactive and Personalized Learning"*. Prof. Srinivas mainly focused on New Education Policy – 2020 and the role of ICT skills in quality and Innovative teaching. He He has explained the aims of NEP – 2020 to create a more engaging, inclusive and learning.

Fourth Session is started at 4: 00 pm. **Prof. K Srinivas** has delivered a lecture in this session entitled *"Designing and Developing Interactive Video content for effective Teaching and Learning"*. In this lecture Prof. Srinivas discussed the challenges and opportunities of ICT platform. He has discuss the advantages of Interactive videos engage learners through dynamic elements.

13

Glimpses of the Day 5 (13th September 2024)

14

15

Report-Day-6 (14/09/2024)

Refresher Course in Computational Science
UGC-MMTTC, Pt. Ravishankar Shukla University – Raipur (C.G.)
Chairman/Reporter: Mr. Shashank Singh Rathore

Session-I (10:30 to 12:00 pm), commenced with a lecture by **Prof. K. Srinivas**, Professor and Head of the ICT and project management unit at the National Institute of Educational Planning and Administration (NIEPA). The session, titled *"Open Educational Resources and Transformative Teaching Learning Practices."* Prof. K Srinivas delivered an engaging talk on the Through the provision of free and easily accessible educational materials to educators and learners globally, Open Educational Resources (OER) are transforming the methods of teaching and learning. Open Educational Resources (OER) facilitates a collaborative, innovative, and inclusive culture by enabling resource customization and sharing to address a range of educational requirements. These materials facilitate the development of adaptable, learner-centred environments that prioritize critical thinking and active learning, so enabling revolutionary teaching approaches. OER is revolutionizing traditional educational models and enabling instructors and students to participate in more significant and lasting learning experiences by lowering obstacles to high-quality education and advancing equity.

Session-II (12:15 to 1:45 pm), was once again led by **Prof. K Srinivas**, session titled **"Exploring Learning Management Systems for enhanced Learning Experiences."** In this session Prof. K Srinivas explained the Enhancing learning experiences in traditional and online education requires the use of Learning Management Systems (LMS), which are essential tools. These platforms give instructors a centralized setting in which to produce, distribute, and oversee communications, assessments, and content. Teachers can create more dynamic and interesting learning experiences by utilizing the features of Learning Management Systems (LMS), such as analytics, multimedia integration, and personalized learning pathways. Additionally, LMS enables flexibility in learning, real-time feedback, and collaboration, meeting the demands of

16

a wide range of learners and enhancing academic results overall. This investigation demonstrates how learning management systems (LMS) have the power to revolutionize education by promoting more effective, flexible, and student-centred learning environments.

Session- III (2:15 to 3:45 pm) commenced with a lecture by **Prof. M.N. Tripathi**, Head, Dept. of Pure & Applied Physics, Incharge-National Center for Accelerator based Research (NCAR) Guru Ghasidas Central Vishwavidyalaya (GGU) Bilaspur (C.G.). The session titled *"Quantum Mechanical Modelling Methods: Genesis and applications."*

Prof. M.N. Tripathi delivered an engaging talk on the Quantum mechanics was first applied to molecules by Erich Huckel gave birth of simple huckel model (SHM) and later extended by Hoffman as extended Huckel model (EHM). These models are based on Schrodinger equation. We will try to understand the genesis of ab initio calculations for electronic structures. This theory does not rely on calibration against measured chemical parameters and give results in terms of fundamental physical constants. We will discuss the importance of Fock operator and physical meaning of quantum mechanical equations to better understand the energy minimisation process and the different terminologies involved. We will explore the fascinating world of material simulation and its different applications for multifunctional materials.

Session-IV (04:00 to 05:30 pm), was led by **Prof. Khemchand Dewangan,** Professor at Department of Chemistry, Guru Ghasidas Central University Bilaspur (CG). His talk, titled *"Fundamentals and Applications of Density Functional Theory."*

Prof. Dewangan discussed Density-functional theory (DFT) is a popular computational modelling approach to calculating the electronic structure of atoms, molecules, and solids. Its goal is the quantitative understanding of material properties from the fundamental laws of quantum mechanics. In the context of the molecular DFT approach, it does not attempt to calculate the molecular wave function but calculates the molecular electron probability density and the molecular electronic energy. Since the electron density is a function of only three-dimensional coordinates, it is also computationally feasible

and affordable for large systems. Therefore, combining DFT approaches with current computers enables accurate calculations in a reasonable time for genuine and exciting molecular systems for scholars in areas as diverse as chemistry, biochemistry, physics, chemical engineering, catalysis, materials science, etc. In this talk, the introduction of DFT and some basic applications will be discussed, which could be helpful to undergraduate and postgraduate students studying physical chemistry in understanding the properties of molecules/atoms.

Glimpses of the Day-6 (14th September 2024)
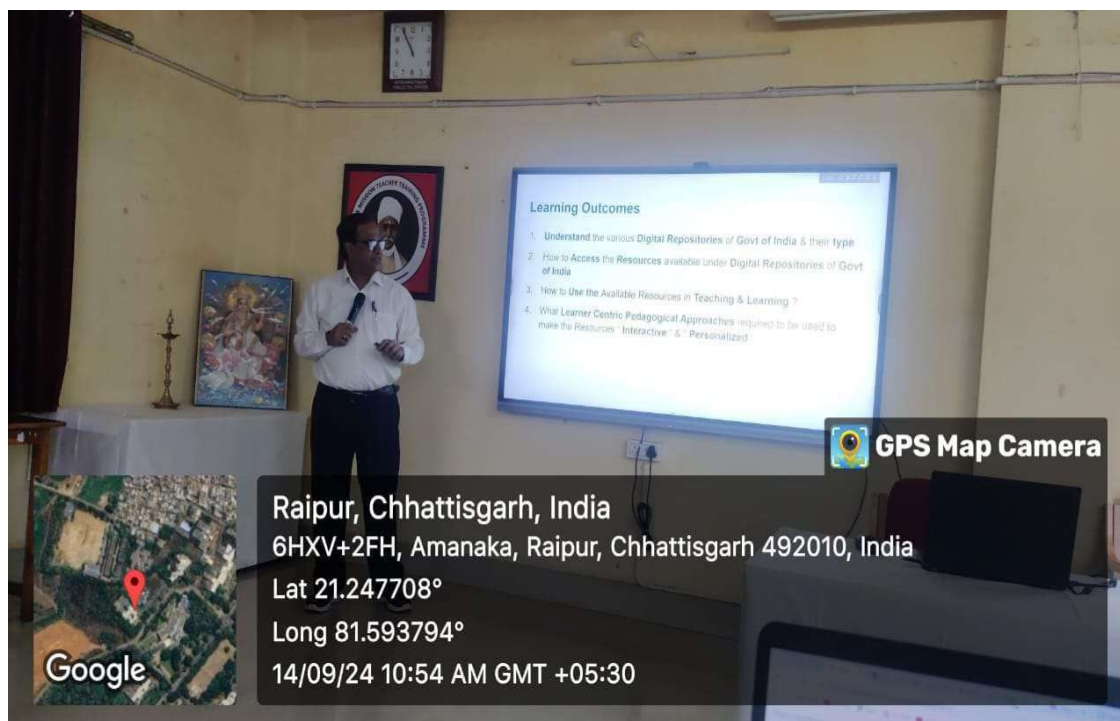
19
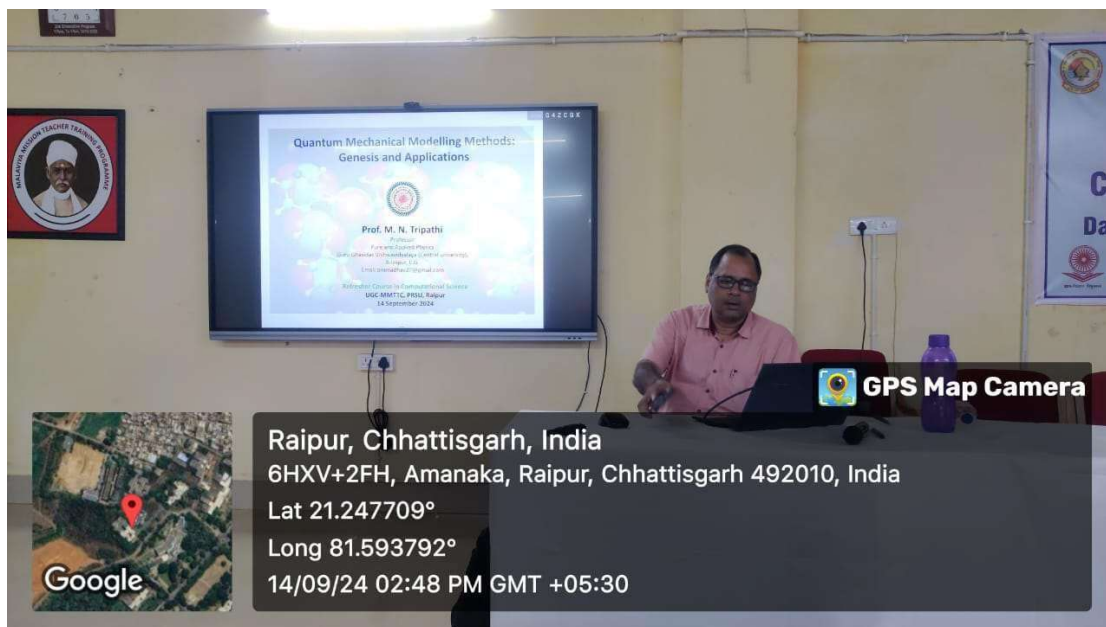
Report-Day-7 (16/09/2024)
Refresher Course in Computational Science
UGC-MMTTC, Pt. Ravishankar Shukla University – Raipur (C.G.)
Chairman/Reporter: Dr. Bhupendra Kumar Sen

Session-I (10:30 am to 12:00 noon), commenced with a lecture by **Prof. M. N. Tripathi,** Head, Dept. of Pure & Applied Physics Incharge-National Centre for Accelerator based Research (NCAR) Guru Ghasidas Vishwavidyalaya (GGU) Bilaspur. The session, titled ***"Designing the materials for desired properties by density functional theory"*** was highly interactive and insightful. Day. In this session Prof. Tripathi demonstrated the Gaussian view software and many hands on preformed for the simple molecules like water, methane, ethane, benzene and trinitro toluene. The energy value for at different dihedral angle and dipole moment can be calculated by the participants on the software. Many other properties like IR frequency, NMR can also be calculated by the Gaussian is demonstrated. Overall, the session was interesting and interactive.

Session-II (12:15 to 01:45 pm), was continued by **Prof. Tripathi** with one more computational software naming material studio which is helpful for the crystal structure. After that he covers the concept of ***Designing the materials for desired properties by density functional theory*** which is exploring recent advancements in analyzing interatomic interactions through quantum mechanical methods, specifically using density functional theory (DFT). DFT has proven to be highly effective in simulating the properties of crystalline solid-state materials, which make up most of these materials. To understand the diverse properties of these substances, a quantum mechanical approach is essential and now feasible. By incorporating various cross-properties and simulating these combined properties with high accuracy, DFT provides valuable insights for designing advanced, efficient materials. In this lecture, Prof. Tripathi cover the process of constructing crystal structures and analyzing the results to understand different material properties. Additionally, participants have hands-on training with photovoltaic and optoelectronic materials to gain a deeper understanding of the simulation processes involved.

Session-III (02:15 to 03:45 pm) was led by **Prof. Sanjay Kumar**, School of Studies in Computer Science & IT, PRSU Raipur, The session, titled **High-Performance Computer: Part-2** was highly interactive and insightful. Prof. Sanjay Kumar started his talk with the importance of computers and various generations of high-performance computing (HPC). He mentions in his lecture as processor technology reached its limits for increasing speed, alternative methods were developed to enhance performance without significantly raising costs or hardware requirements. One effective method is **pipelining**. Pipelining boosts throughput and speed by allowing multiple stages of processing to overlap, akin to an assembly line where each stage works simultaneously on different parts of a task. To improve processor speed, several techniques are utilized:1. **Increasing clock speed, 2. Widening the data bus and 3. Pipelining.** Pipelining involves breaking down a process into distinct stages that can be executed in parallel. For example, in offline counselling for admissions, different stages like reporting, document verification, merit preparation, and seat allotment can overlap, keeping each stage continuously occupied. The lecture has covered the principles of pipelining, its various types, and its implementation, providing insights into how pipelining can be optimized for better performance.

Session-IV (04:00 to 5:30 pm) was led by **Prof. O P Vyas**, Department of Information Technology, IIIT Allahabad, Allahabad (UP), The session, titled **"Foundations of Process Science: Process Modelling"** was highly interactive and insightful. He discussed that "Foundations of Process Science: Process Modelling" introduces the essential concepts and principles underlying process modelling, a critical aspect of process science. Prof. Vyas session explore how process modelling serves as a blueprint for understanding, analysing, and optimizing organizational processes. He Said that by focusing on the systematic representation of processes, participants could gain insights into how models facilitate the visualization of complex workflows, support decision-making, and ensure alignment with organizational goals. The session was underscore the importance of accurate and robust process models as foundational tools in the broader scope of process science. The complete session was interactive in insightful for all the participants.

The Session ended with vote of thanks by Dr. Bhupendra Kumar Sen (Chairman)

Glimpses of the Day 7 (16th September 2024)
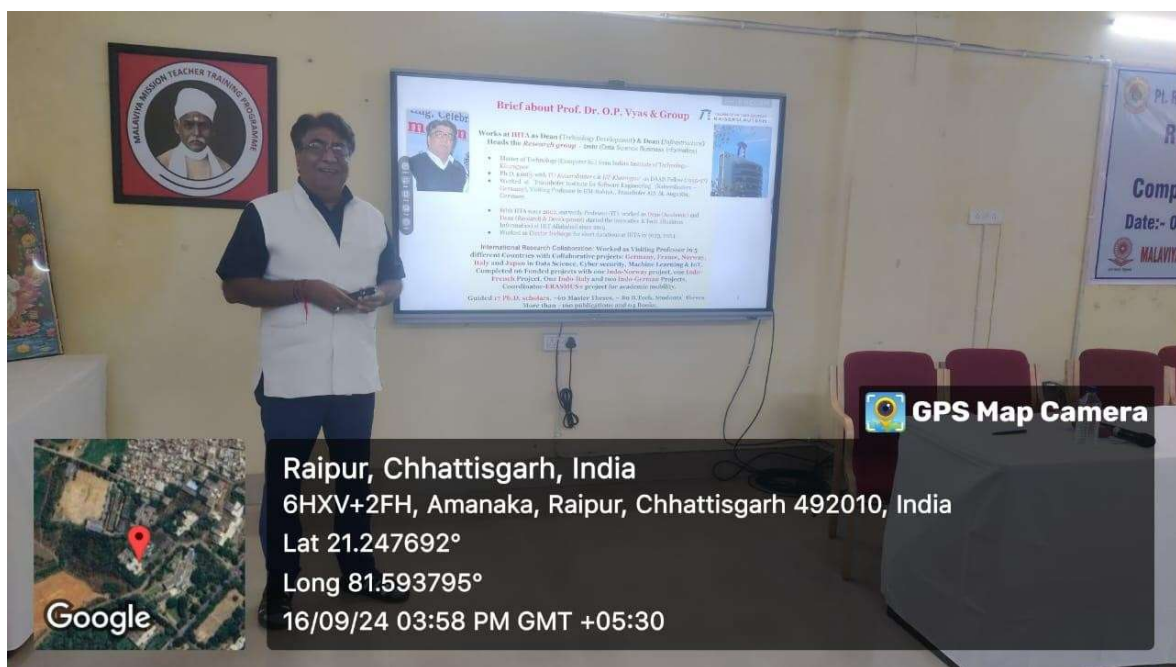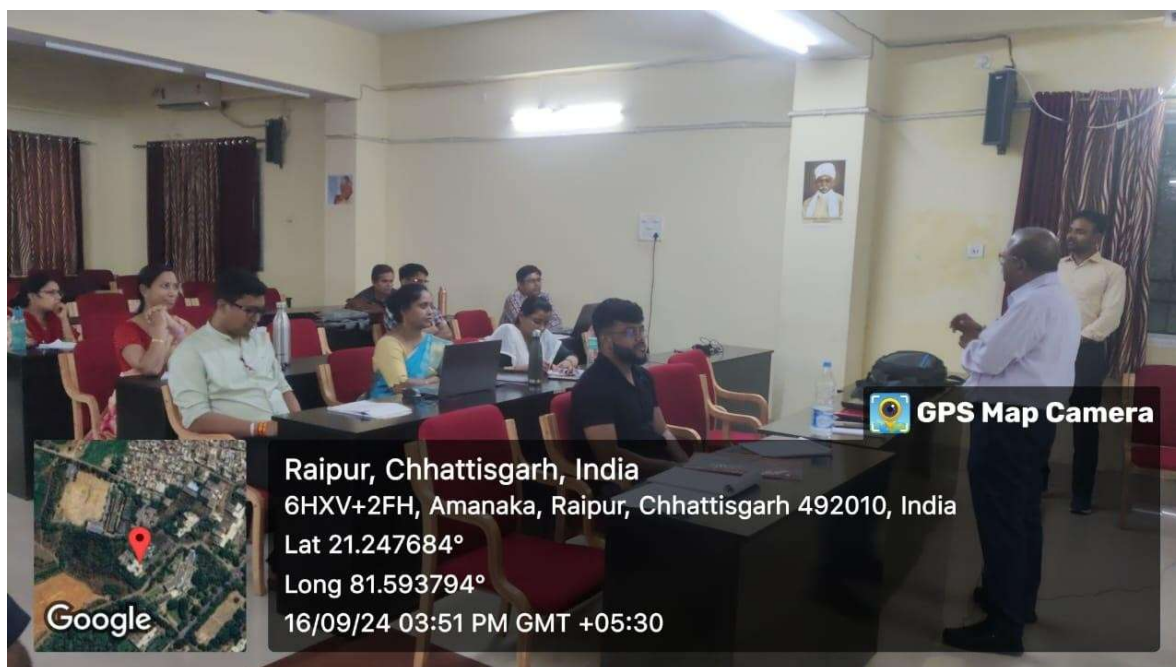
Report-Day-8 (18/09/2024)
Refresher Course in Computational Science
UGC-MMTTC, Pt. Ravishankar Shukla University – Raipur (C.G.)
Chairman/Reporter: Dr. Bhanushree Gupta

Session-I (10:30 to 12:00 noon) commenced with the lecture of **Professor Kamlesh Kumar Shriwas, School of Studies in Chemistry, Pt Ravishankar Shukla University, Raipur.** He delivered his talk on **"Role of Statistics in Computational Science and Scientific Research".** He discussed how statistics can be correlated with day to day life and how does it make our life easier. Further he explained some basic concepts of analytical chemistry viz. accuracy, precision, various tests like F- test, t- test, chai test etc. He also discussed ANOVA and its types (one way, two way). Prof. Shriwas also gave some mathematical problems on significant figures, standard deviation to solve and made the session interactive. The session concluded with an engaging question-and-answer round.

Session-II (12:15 to 13:45 pm) and **Session-III** (02:15 to 03:45 pm)- **Seminar** was organized for the participants in both the sessions. **Prof. Manas Kanti Deb, Director, Natural Center for Natural Resources and School of Studies in Chemistry, Pt Ravishankar Shukla University, Raipur** evaluated the sessions. The theme of the seminar was based on Computational Sciences. Total 10 participants presented in both the sessions of Seminar. Each participant was given 10 mins of time for presentation followed by 2mins for question-answer session. The details of participants who presented along with title of their seminar are given below.

S. No.	Name of Participants	Title
1.	Mr. Chitrkant Belodhiya	Cloud Computing
2.	Dr. Swati Jain	Cyber Security
3.	Dr. Bhupendra Sen	Role of Computational Sciences in Chemistry
4.	Mr. Dildar Singh Tandon	Application of Computational Sciences in Mathematics
5.	Dr. Govind Prasad Sahu	The future of Computational Sciences

6.	Mr. Shashank Rathore	DFT method
7.	Dr. Yugal Kishore Mahipal	Green Computing and Sustainability
8.	Dr. Indrapal Karbhal	Chat GPT
9.	Mr. Lokesh Satpathi	Artificial Intelligence
10	Dr. Bhanushree Gupta	Role of AI in Drug Discovery and Development

**Session-IV** (16:00 to 17:30 pm) was led by **Dr. Vinod Kumar Patle, Associate Professor, School of studies in Computer Sciences and Technology. He delivered his talk on "New Paradigm of Information Technology"**. Dr. Patle discussed how information technology is helpful in our daily routine and related it with all important sectors like banking, communication, health and wellness, entertainment, travel and navigation etc. He further discussed the role and impact of Artificial Intelligence in our life.

He explained various types of computing like cloud computing, edge computing, quantum computing and digital platforms with their applications in details. He wonderfully explained the IoT (internet of things). He highlighted the role of IT in new education policy too. Participants were given the opportunity to interact with Dr Patle for their queries. Finally the session was concluded with vote of thanks given by chairman of the day.

24

Glimpses of the Day 8 (18ᵗʰSeptember 2024)

25

26
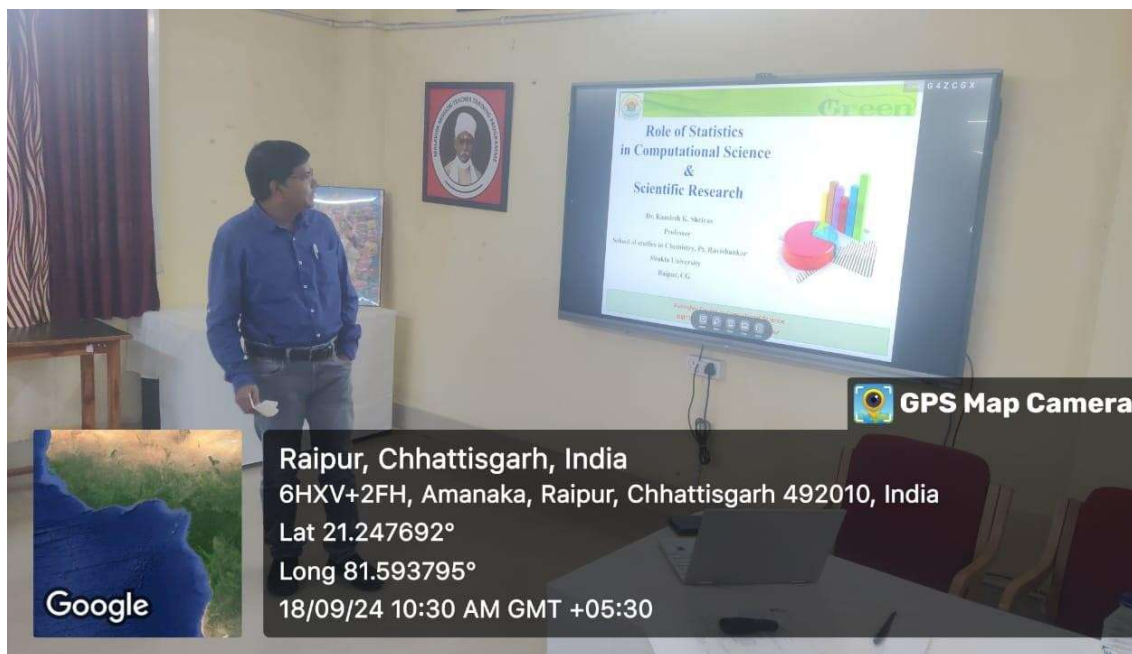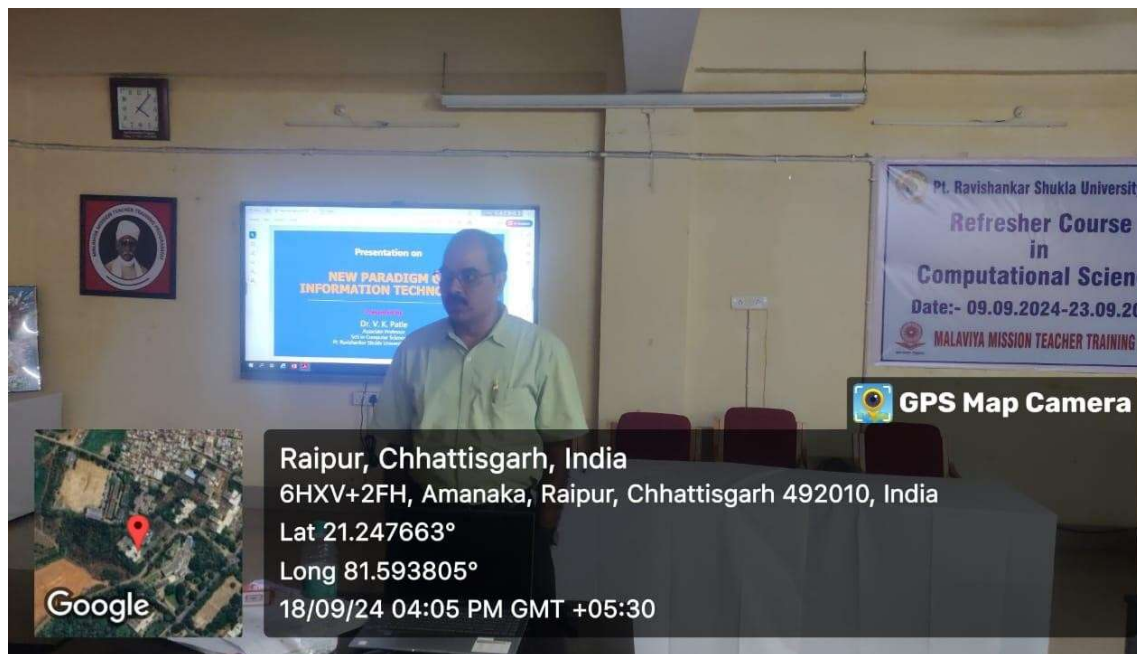
Report-Day-9 (19/09/2024)
Refresher Course in Computational Science
UGC-MMTTC, Pt. Ravishankar Shukla University – Raipur (C.G.)
Chairman/Reporter: Mr. Lokesh Satpathi

The first session on the 9th day of the refresher course began at 10:30 a.m. **Dr. Md. Mehboob Alam**, an Assistant Professor in the Department of Chemistry at IIT Bhilai, delivered a lecture on *"Basic Quantum to Computational Methods."* Dr. Alam started with a brief story about Professor Mukherjee, an experimental chemist, at Kolkata university highlighting the transformative impact of the computer revolution in science. He discussed the power of computational tools and their multidisciplinary applications.The lecture covered fundamental topics such as quantum mechanical *ab initio* methods and basic quantum mechanics. Dr. Alam explained the Born-Oppenheimer approximation and engaged participants in discussions on the Hartree-Fock approximation and an introduction to basis sets. He also elaborated on the Hartree-Fock algorithm and the processes involved.The session concluded with a lively question-and-answer interaction, allowing participants to further explore the subject matter.

The second session of the day started at 12:15 p.m., led by **Dr. Md. Mehboob Alam**. This was a hands-on session focused on quantum mechanical simulations for predicting the optical properties of materials. Dr. Alam also discussed vibrational spectroscopy, particularly infrared (IR) spectroscopy, and guided participants through a hands-on exercise using open-source software tools like DALTON and ORCA. He explained the features and applications of these tools in detail, emphasizing their utility for teaching purposes.The session was successful, with participants gaining practical insights into using computational software for quantum mechanical simulations.

The third session was a seminar session chaired by **Professor Manas Kanti Deb** from the Department of Chemistry, Pt. Ravishankar Shukla University, Raipur. Ms. Shail Sharma, Mrs. Vaishnavi Mandavi, Dr. Deena Sunil, and Ms. Megha Sahu presented their seminar lectures during this session. At the end of the session, Professor Manas Kanti Deb gave a brief concluding note. He spoke about the early days of the Department of Chemistry, providing insights into its history, and discussed the advancements in technology that have made tasks such as online banking and other activities more convenient today. He emphasized how these advancements have transformed the way research and work are conducted.

The session concluded with a vote of thanks to Professor Manas Kanti Deb for chairing the session.

The fourth session of the day featured a talk by **Professor Balwant Singh Thakur** from the School of Studies in Mathematics, Pt. Ravishankar Shukla University, Raipur. The topic was *"Research Impact in Computational Sciences: Understanding Journal Impact Factor and Author Metrics."*

The session was highly interactive and useful for all participants. Professor Thakur discussed key aspects of research, including what constitutes a research journal, the concept of impact, tracking and measuring impact, and the role of discipline-specific metrics like Altmetrics. He also elaborated on various journal citation systems and provided insights into the history and significance of citation indexes, journal impact factor (JIF), and Google Scholar. He explained important concepts like the difference between references and citations, GIF (General Impact Factor), GCR (Global Citation Ranking), and Source Normalized Impact per Paper (SNIP).Professor Thakur shared details about the founders of Google and explained how the platform has become an invaluable tool for researchers. The session ended with a question-and-answer discussion, where participants actively engaged and benefited from the insights shared by Professor Thakur.

Finally, Mr. Lokesh Satpathi Chairperson of the Day thanked the participants and Professor Balwant Singh Thakur, bringing the session to a close.

Glimpses of the Day 9 (19ᵗʰSeptember 2024)

29
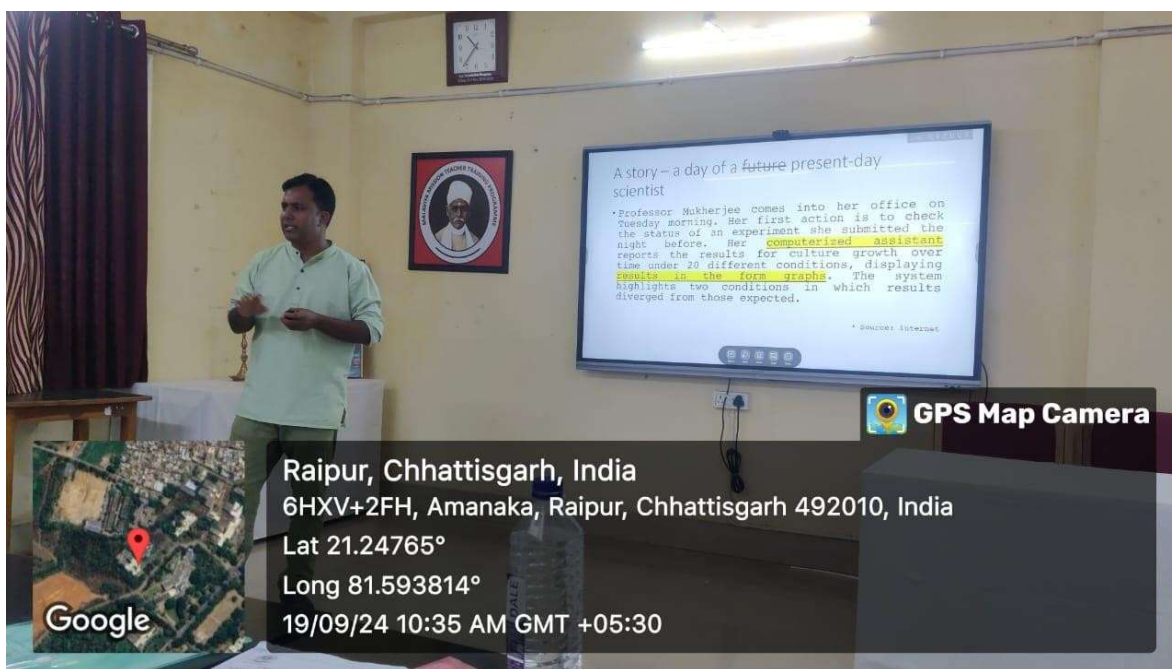
Report-Day-10 (20/09/2024)
Refresher Course in Computational Science
UGC-MMTTC, Pt. Ravishankar Shukla University – Raipur (C.G.)
Chairman/Reporter: Dr. Deena Sunil

The **first session** of the tenth day of the refresher course started at 10.00 am on 20-09-2024. **Dr. Vinod Kumar Patle,** School of Studies in Computer Science, Pt. Ravishankar Shukla University, delivered an insightful lecture on "Moodle." Moodle is a free and open-source learning management system written in PHP and distributed under the GNU General Public License. Moodle is used for blended learning, distance education, flipped classroom and other online learning projects in schools, universities, workplaces and other sectors.

The **second session** of the tenth day of the refresher course started at 2.00 pm on 20-09-2024. **Prof. Gourisankar Roy Mahapatra,** Department of Chemistry, Haldia Institute of Technology, Haldia. He discussed the key elements involved in writing an effective project, focusing on the structure, methodology, and essential components required for crafting a successful project proposal. He emphasized the importance of clarity in defining objectives, outlining the scope, and presenting a comprehensive literature review to support the project's significance. He evaluate our project work.

Report-Day-11 (21/09/2024)
Refresher Course in Computational Science
UGC-MMTTC, Pt. Ravishankar Shukla University – Raipur (C.G.)
### Chairman/Reporter: Shail Sharma

The first session of the eleventh day of the refresher course started at 10:30 am on 21-09-2024.

Dr. Md. Mehboob Alam, Assistant Professor in Department of Chemistry, **Indian Institute of Technology (IIT) Bhilai**, delivered an insightful lecture on Basics of Molecular Dynamics and Genetic Algorithm. He explained types of molecular dynamics as well as he discussed about the total energy calculation of this type of system. He elaborated the calculation of different potentials which exits in molecular dynamics. One of the methods is EAM. Also he described to the audience that predictor-corrector algorithm and Verlet algorithm can be used for solving the Newton's equations of motion in molecular dynamics simulation. Throughout the lecture, Dr. Md. Mehboob Alam explained these concepts in a simple, approachable manner.

The second session started at 12:00 pm and once again led by **Dr. Md. Mehboob Alam** who conducted a hands-on training session titled " Hands-on Molecular Dynamics Simulation". In this session Dr. Alam demonstrated that how to use Gaussian and LAMMPS software. Using this software, participants were given the opportunity to perform hands-on exercises on several key ingredients of molecular dynamics simulations, such as system initialization, energy minimization, integration of the equations of motions and trajectory visualization.

31
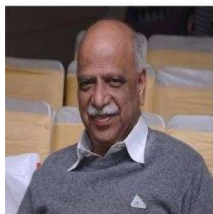
The third session started at 02:15 pm and was led by **Prof. Shridhar R. Gadre, Bhatnagar Awardee, INSA Senior Scientist at Department of Scientific Computing, Modelling and Simulation & Department of Chemistry, Savitribai Phule Pune University.** The session, titled **"Storage of Numbers in a Computer, Roundoff Errors, Truncation Errors…"** was based on basics of numbers systems which are used in scientific computing software. He explained Computers can only represent a finite number of distinguishable values. There are many different ways to represent numbers on computers, all with different strengths and weaknesses. The range of representable numbers depends on the size of memory allocated to store it. He briefly explained the conceptual difference of "**Real Line**" in mathematics and computer. He also elaborated double, quadruple precision and round-off, truncation errors with some examples. Awareness about these errors is essential for developers and users of scientific computing software.

The fourth and last session of the day started at 4:00 pm. In this session, a MCQ test was conducted for participants according to the guideline provided by the UGC HRDC, in the guidance of Course Coordinator Prof. Kallol K. Ghosh, Head, SoS in Chemistry, Pt. Ravi Shankar Shukla University, Raipur.

Glimpses of the Day 11 (21ˢᵗ September 2024)
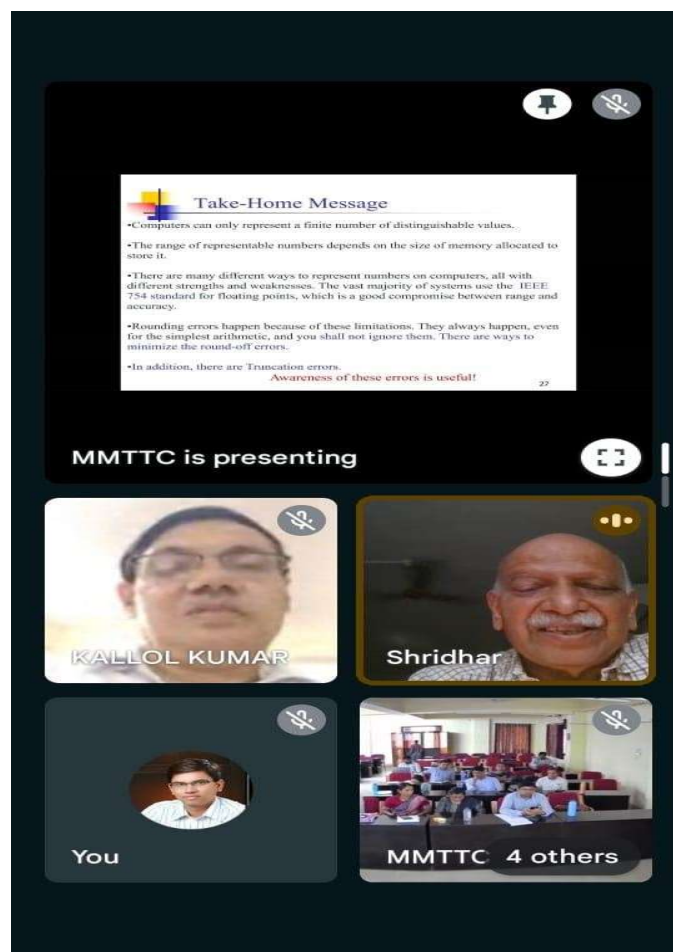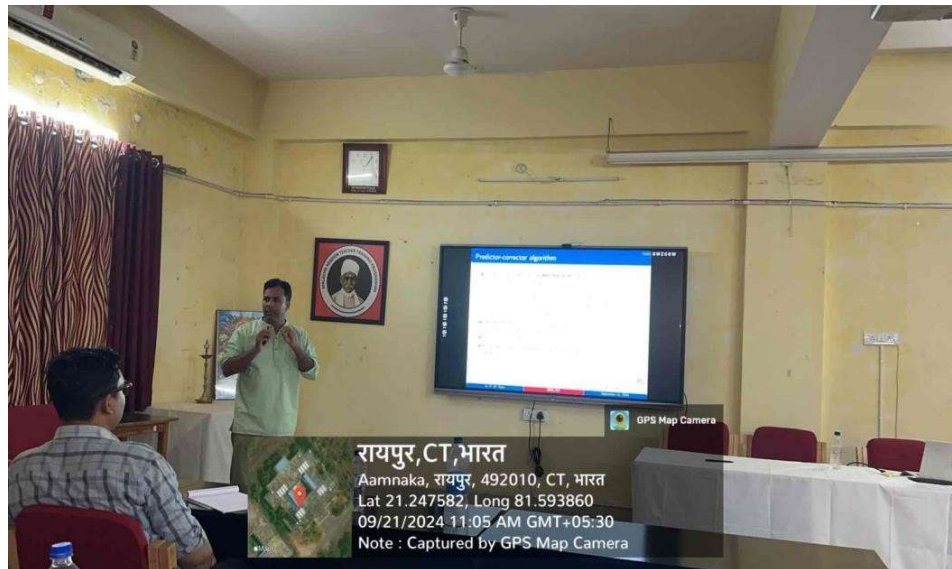
Report-Day-12 (23/09/2024)
Refresher Course in Computational Science
UGC-MMTTC, Pt. Ravishankar Shukla University – Raipur (C.G.)
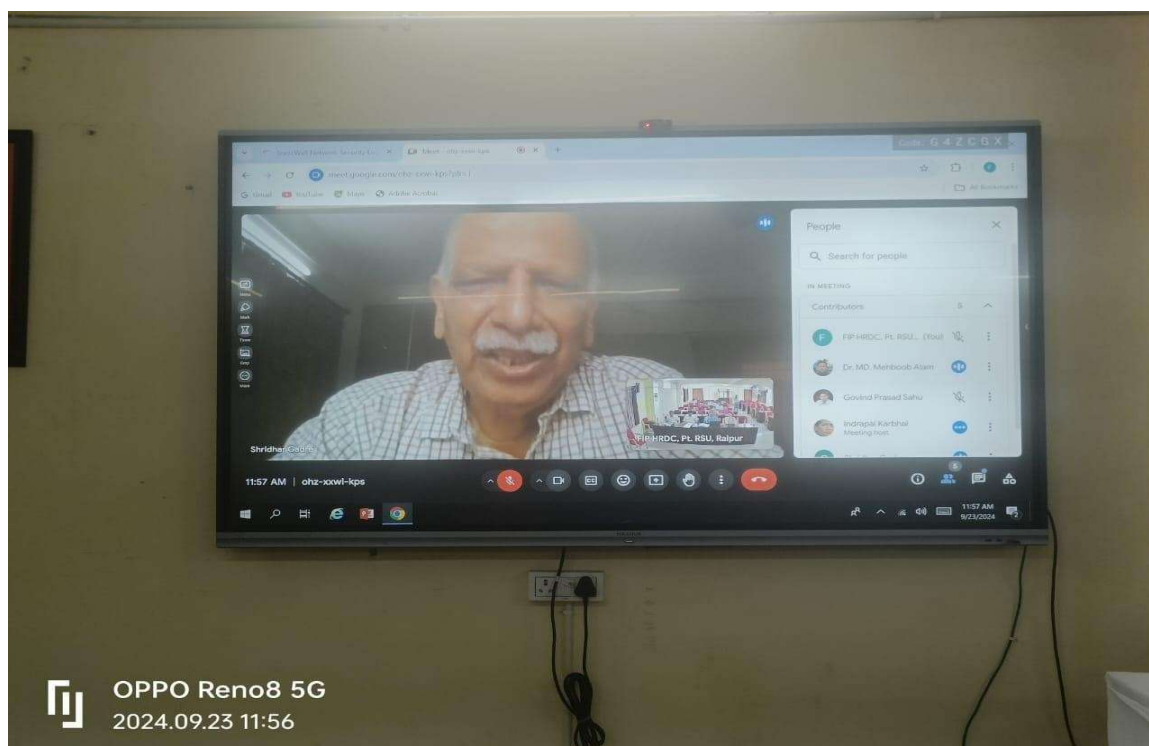### Chairman/Reporter: Vaishnavi Mandavi

Session-I (10:30 to 12:00 noon) commenced with the lecture of **Professor Shridhar R. Gadre**, Bhatnagar Awrdee. Professor Shridhar R. Gadre from Savitribai Phule Pune University delivered an insightful lecture on indigenous quantum chemistry algorithm and code development. The first session focused on the "Molecular Tailoring Approach (MTA)" for handling large molecular systems in computational chemistry. Gadre highlighted the significant challenges of quantum chemical calculations, especially for large molecules, due to the exponential growth of computational requirements. His research group developed MTA to tackle these issues by fragmenting large molecules into smaller, computationally manageable parts. These fragments are then analyzed, and the results are recombined using set theory principles to approximate the properties of the entire molecule. This approach has enabled highly accurate energy and property calculations while reducing the computational complexity.

Gadre also discussed the advancements in hardware and software over the years, emphasising the importance of collaboration between academia and industry. He explained that the MTA method, initially conceived in 1994, has been refined over the years to incorporate modern computational techniques like Python scripting and distributed computing, which have vastly improved its efficiency and applicability. Moreover, the accuracy of MTA for geometry optimization and vibrational spectra calculations has been validated against high-level quantum mechanical methods, making it a valuable tool for studying molecular clusters and biomolecules. Gadre's work has played a crucial role in advancing computational chemistry in India, supporting the Atma Nirbhar Bharat mission by fostering self-reliance in scientific computing.

In the second session, a valedictory function was organized, Course coordinator **Prof. Kallol K. Ghosh**, MMTTC Director **Prof Preeti Suresh** and Course -Coordinator from MMTTC, **Dr. Arvind Agrawal** were present in this session. At the very outset course coordinator Prof. Kallol K. Ghosh extended a warm welcome to all the participants of the course. He briefly presented the report of the Refreshers Course on Computational Science and

discussed the important topics covered in this course. He also appreciated the cooperation and support received from the MMTTC Centre. Some participants shared their feedback regarding the refresher course. The director of the MMTTC Prof. Preeti K. Suresh finally expressed her view on this extremely useful interdisciplinary refresher course. The session ended with a vote of Dr. Arvind Argrawal.

<p align="center">**Glimpses of the Day 12 (23rd September 2024)**</p>