

Online Faculty Development Programme (FDP) on **Cultivating Excellence in Implementation of Computational Science for Scientific and Technological Innovations**



June 14th - 18th 2021

Hosted Online



Organised by

Department of Metallurgical and Materials Engineering

National Institute of Technology, Rourkela

<http://cpcm2020.com/>

Patron



Prof Animesh Biswas
Director, NIT Rourkela

Head of Department



Prof. Anindya Basu
Dept of Metallurgical and
Material Engg

Program Coordinator



Dr. Snehanshu Pal
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About NIT Rourkela

National Institute of Technology Rourkela (NITR), formerly Regional Engineering College Rourkela (REC Rourkela), established in 1961, is one of the premier national level institutions for technical education in the country and is funded by the Government of India. As per the Times Higher Education World University Rankings of 2021, NIT Rourkela has the position in between 801-1000 in the world and 190th in Asia. QS BRICS overall University Ranking 2019 has figured NIT Rourkela at 121st position. NIT Rourkela is presently ranked the 3rd best NIT and 16th nationwide (including IITs) by the MHRD. The campus has all the amenities for developing personal, social and academic skills of the student community. The Institute has been modernized by two foreign collaborative funding agencies i.e. the Material theme in the Materials and Metallurgical Engineering department under Indo-U.K. REC project and the Computer Science and Electronics streams under World Bank cum Swiss Development Corporation IMPACT project. With 21 departments awarding graduate and post graduate degrees including Ph.D. in Engineering, Science, Planning and Architecture, Management, and Humanities, NIT Rourkela is one of the prestigious institutes in the country. NIT Rourkela is a well-known technical institute of national importance serving as a knowledge hub to the nation. The campus of the institute consisting of the Institute buildings, halls of residence and staff colony, spread over an area of 262 hectares of land is surrounded by scenic hills providing a spectacular rejuvenating atmosphere, which is very conducive for study and research. The well maintained green campus of the Institute provides accommodation to all students, faculties and staffs. The campus has all the amenities for developing personal, social and academic skills of young people. The greeneries and flowers in the campus further make the stay very pleasant and enjoyable.

About Department of Metallurgical and Materials Engineering

Established in 1964, the Department has emerged as a powerhouse for academics, scientific research, and cutting-edge technologies. With time, the department grew noticeably and established new areas of research and teaching in materials engineering, while retaining its strength in traditional areas of metallurgical engineering. The department is actively involved in fundamental research in diversified fields like steel technology, advanced manufacturing processes, alloy designing, nanotechnology, composites and computational materials. The alumni of the department hold strong positions in many prestigious organizations over the world. The department attracts highly qualified faculties and bright students from the entire nation. The well-developed infrastructure, diversified expertise of the faculties and incredibly talented students has placed the department in the global forum. The graduates from the department are well-placed in esteemed industries and institutions. The department has a history of producing highly ambitious students motivated for higher education in India and overseas. The department is actively involved in research activities in the front line areas of Metallurgical and Materials Engineering in collaboration with reputed R&D organizations and industries throughout the country. The research wing of the department is strongly supported by various public and private organizations. At present, various research projects are being run in the department by external sponsoring agencies like Department of Science and Technology (DST), Council of Scientific and Industrial Research (CSIR), Naval Research Board (NRB), Defence Research and Development Organisation (DRDO), Board of Research in Nuclear Sciences (BRNS), National Aluminium Company (NALCO), TATA Steels, Steel Authority of India Ltd (SAIL). Metallurgical and Materials Engineering Department of NIT Rourkela has a strong and gracious history of organizing technical national/international conferences, workshops and short term courses. This department has been organizing the conference every year in the month of December since 2011 and the conference becomes well known among students, young researchers, material scientists and academicians.

Profile of the Program Coordinator

Dr. Snehanshu Pal is currently working as an assistant professor in Department of Metallurgical and Materials Engineering, National Institute of Technology Rourkela. He has served as Post-Doctoral Fellow Department of Materials Science and Engineering, The Pennsylvania State University, USA. He has done Ph.D. in Metallurgical and Materials Engineering from Indian Institute of Technology, Kharagpur, India. He is leading the Computational Materials Engineering and Process Modelling Research Group at NIT Rourkela, and a group dedicated to realizing the underlying physics behind the mechanical behaviour of materials and simulating metallurgical processes (<http://www.snehanshuresearchlab.org>). He has published seventy three high-impact research articles in internationally reputed SCI indexed journals. He has authored two books (Title: “Molecular Dynamics Simulation of Nanostructured Materials”, Publisher: CRC Press) and (Title: “Process Modelling for Steel Industry”, Publisher: IK International). He has supervised five doctoral theses and several master theses. He is an investigator of five sponsored research projects and industrial projects. In addition, Dr. Snehanshu Pal is associated with various esteemed technical and scientific societies such as Indian Institute of Metals and Indian Institute of Engineers. Recently, he has organized online workshop as a coordinator (“Molecular Modelling of Materials and Biological Macro Molecules” dated 22 Sep 2020 - 26 Sep 2020), one online conference as a convener (“Conference on Processing and Characterization of Materials (CPCM 2020)”, dated 18 Dec 2020 - 20 Dec 2020).

Target Participants

- Faculties of Engineering and Science Colleges interested in teaching and performing research in
 - i) Computer science
 - ii) Computational Chemistry
 - iii) Computational Physics
 - iv) Computational Biology
 - v) Computational Engineering
 - vi) Computational Nano material
- Advanced Post-Graduate Students and research scholars in Science and Engineering.

About the workshop

Computational Science have become an essential part of different streams of sciences and engineering. Computational techniques are not only confined within the advanced field of modern research but also have taken place in the curriculum of the undergraduate levels. The 5-days workshop would provide essential information on the basics of Computational Science and associated techniques to the faculties and young researchers who want to gain experience in the areas of implementing computational techniques to solve scientific/technical problems and bring innovation in science, engineering technology. The tutorial/hands on session of the workshop will cover the basic principles and advance computational techniques to determine various technical problem and will introduce basics of length and time scales challenges through simulations. Significantly there will be a session on “science and spirituality” in this program.

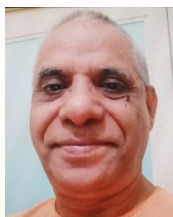
Program Content

1. Uncertainty modeling in Engineering and Technology.
2. Digital stochasticity in scientific computing.
3. Cyber security and associated risk management.
4. Opportunities of Numerical Simulation in Corrosion technology.
5. Application of Density Function Theory toward Innovation in Material Science/Technology.
6. Inverse Materials Design Through Computation.
7. Analyzing the driving forces of protein stability in presence of co-solvents.
8. Materials Modelling using First-Principle calculations.
9. Computational perspective of *Oxide dispersion strengthened alloys (ODS alloys)* development.
10. Robotic Process Automation-(What, Why, When and How)
11. Hands on Machine learning using Python.
12. Hands on atomistic simulation using Lammmps Platform.
13. Science, Spirituality and Self-transcendent emotions.
14. Assessment and Feedback.

Program Schedule

14th June 2021 Monday	Inauguration (9:00 am—9:30 am)		
14th June 2021 Monday	Session 1 (9:30 am -11:30am) Uncertainty modeling in Engineering and Technology Resource Person: Dr. Snehashish Chakraverty	Session 2 (11:30 am - 1:30pm) Digital stochasticity in scientific computing Resource Person: Dr. Amlan Dutta	Session 3 (3:30 pm -5:30pm) Scope of Molecular Dynamics in Materials Engineering Resource Person: Dr. Snehanshu Pal
15th June 2021 Tuesday	Session 4 (9:30 am -11:30am) Opportunities of Numerical Simulation in Corrosion technology Resource Person: Dr. Archana Mallick	Session 5 (11:30 am -1:30pm) Application of Density Function Theory toward Innovation in Material Science/Technology Resource Person: Dr. Tarun Kumar Kundu	Session 6 (3:30 pm– 5:30 pm) Inverse Materials Design Through Computation Resource Person: Dr. Gautam Anand
16th June 2021 Wednesday	Session 7 (9:30 am -11:30am) Analyzing the driving forces of protein stability in presence of co-solvents Resource Person: Dr. Madhurima Jana	Session 8 (11:30 am -1:30pm) Materials Modelling using First-Principle calculations Resource Person: Dr. Debolina Misra	Session 9 (3:30 pm -5:30pm) Computational perspective of Oxide dispersion strengthened alloys (ODS alloys) development Resource Person: Dr. Anshuman Patra
17th June 2021 Thursday	Session 10 (9:00 am -11:00am) Cyber security and associated risk management Resource Person: Dr. Ruchira Naskar	Session 11 (1:00 pm -3:00pm) Robotic process automation - (What, Why, When and How) Resource Person: Dr. Madhushi Verma	Session 12 (3:30 pm -5:30pm) Hands-on: Geospatial Data Analysis using Supervised and Unsupervised Classification Technique Resource Person: Er. Urvashi Nag
18th June 2021 Friday	Session 13 (9:30 am -11:30am) Science, Spirituality and Self-transcendent Emotions Resource Person: Swami Buddhadevananda	Session 14 (11:30 am -1:30pm) Hands-On: Application of Machine Learning Techniques in Materials Engineering Sector Resource Person: Dr. Amitava Choudhury	Session 15 (3:00 pm -5:30pm) Assessment, Feedback and Valedictory

CONFIRMED RESOURCE PERSON



Swami Buddhadevananda
Secretary
Ramakrishna Mission, Rourkela



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Indian Institute of Engineering
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Registration and workshop venue

There is no registration fees. Interested candidate has to register in the link given below. Last date of registration is 5th June 2021.

Maximum 200 participants only.

Registration link: <https://atalacademy.aicte-india.org/>

Venue: NIT Rourkela, Online mode. Meeting link will be shared to the registered participants



Our
Institute

