NATIONAL INSTITUTE OF TECHNOLOGY
ROURKELA

WORKSHOP ON
MOLECULAR MODELING
OF MATERIALS
& BIOLOGICAL
MACROMOLECULES

2020

SPONSORED BY TEQIP-III

- **Registration Opens till 20th Sep, 2020**

Link: https://forms.gle/zoTZP4uV8udZ5EMw6

- **Webinar Workshop duration**

22-September-2020 to 26-September-2020

OUR PATRON — **Prof. Animesh Biswas, Director, NIT Rourkela**

COORDINATOR OF TEQIP-III — **Prof. Chittaranjan Patra, Civil Engg. Dept.**

HEAD OF THE DEPARTMENT — **Prof. Anindya Basu, Dept of Metallurgical and Material Engg.**
Prof. Rupam Dinda, Dept. of Chemistry

OVERVIEW / OBJECTIVES

Molecular modeling and molecular simulations have become an essential part of different streams of sciences and engineering. Such 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 molecular modeling techniques to the faculties and young researchers who want to gain experience in the areas of molecular modeling including biological, physical and chemical sciences, metallurgical and material engineering.

The tutorial session of the workshop will cover the basic principles and advance simulation techniques to determine various physicochemical properties in materials science and will introduce basics of length and time scales challenges, atomistic, *ab-initio* and coarse-grained simulations etc.

PROGRAM CONTENT:

- Atomic scale materials modeling
  - Tutorial session using VASP
  - Tutorial session using Materials Studio
- Modeling and simulations of bio macro molecules
  - Tutorial session using AMBER and NAMD
- Electronic structure theory based modeling
  - Tutorial session using GAUSSIAN program: Optimization, UV spectra, NMR properties; Input files preparation and analysis of results.
- Discussion with the panel members

CONFIRMED SPEAKERS

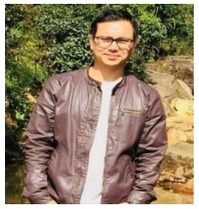
Prof. Sourav Pal
Director
IISER Kolkata

Prof. Tarun K Kundu
Dept of Metallurgical and Material Engg.
IIT Kharagpur

Prof. Debesh R Roy
Dept. of Applied Physics
SVNIT Surat

Dr. Kaushik Chakraborty
Senior Scientist, CubeBio AI
PES University, Bangalore

Dr. Rajeev R
Dept of Chemistry
NIT Rourkela



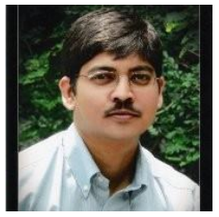
Dr. Sourab Sinha
SCUBE, New Delhi

Prof. Swapan K Pati
Chairman, Theoretical Sciences Unit
JNCASR Bangalore

Prof. Srabani Taraphder
Dept. of Chemistry
IIT Kharagpur

Prof. Subash Ganguly
Dept of Metallurgical and Material Engg.
NIT Raipur

Dr. Jay Chakraborty
Scientist
NML, Bhubaneswar



Dr. Ritwik
Dassault Systems Ltd., Bangalore

TENTATIVE BRIEF SCHEDULE

Date	9 AM - 12:00 Noon	
Day-1 22-September-2020	• Inauguration • Keynote speech-I : Prof. Sourav Pal • Keynote speech-II: Prof. Swapan K Pati	
Day-2 to Day-5	**First Session (9:30 AM – 11:30 AM) Invited Lectures/Tutorials/Discussion**	**Second Session (3:00 PM – 5:00 PM) Invited Lectures/Tutorials/Discussion**
23-September-2020	Prof. Tarun K. Kundu	Prof. Srabani Taraphder
24-September-2020	Prof. Subash Ganguly	Prof. Debesh R. Roy (Talk + Tutorial)
25-September-2020	Dr. Jay Chakraborty	Dr. Kaushik Chakraborty (Talk + Tutorial)
26-September-2020	Dr. Sourab Sinha (Tutorial)	Dr. Rajeev R (Talk + Tutorial) Dr. Ritwik (Tutorial)

TARGET PARTICIPANTS

Faculties of Engineering and Science Colleges interested in teaching Computational Chemistry, Computational Physics, Computational Biology, Computational Metallurgical and Materials Sciences and Engineering, Computational Nanomaterial; Advanced Post-Graduate Students in Science and Engineering. Number of participants is limited to 100.

CERTIFICATE:

e-certificate will be provided to the registered participants at the end of the entire workshop.

REGISTRATION & WORKSHOP VENUE:

There is no registration fee. Interested candidate has to fill up the Google form. **Last date of Registration: 20th September, 2020. Registration LINK: https://forms.gle/zoTZP4uV8udZ5EMw6.**

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

WORKSHOP COORDINATORS & CONTACT DETAILS:

Dr. Madhurima Jana
Dept. of Chemistry
NIT Rourkela
Email: madhurima.mml@gmailcom
Contact No: 9556353217

Dr. Snehanshu Pal
Dept. of Metallurgical and Materials Engineering
NIT Rourkela
Email: snehanshu.cms@gmail.com
Contact No: 8895540586