



**WORKSHOP ON  
MOLECULAR MODELING  
OF MATERIALS  
& BIOLOGICAL  
MACROMOLECULES**

**2020**

**SPONSORED BY**

**TEQIP-III**





- Registration Opens till **20<sup>th</sup> 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



## 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, 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



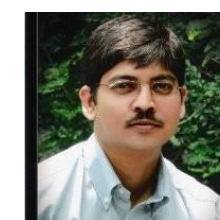
Prof. Srabani Taraphder  
Dept. of Chemistry  
IIT Kharagpur



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



Dr. Jay Chakraborty  
Scientist  
NML, Jamsedpur



Dr. Ritwik  
Dassault Systems  
Ltd., Bangalore



Dr. Debolina Misra  
Dept of Metallurgical and Material Engg.  
IIT Madras

## 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

## TENTATIVE BRIEF SCHEDULE

Date	2 PM - 4:45 PM	
Day-1 22-September-2020	<ul style="list-style-type: none"><li>• Inauguration</li><li>• Keynote speech-I : Prof. Sourav Pal</li><li>• Keynote speech-II: Prof. Swapan K Pati</li></ul>	
Day-2 to Day-5	<b>First Session (9:30 AM – 11:30 AM)</b> <b>Invited Lectures/Tutorials/Discussion</b>	<b>Second Session (3:00 PM – 5:00 PM)</b> <b>Invited Lectures/Tutorials/Discussion</b>
23-September-2020	Prof. Tarun K. Kundu (IL-1) Dr. Debolina Misra (Tutorial)	Prof. Srabani Taraphder (IL-2)
24-September-2020	Prof. Subash Ganguly (IL-3)	Prof. Debesh R. Roy (IL-4 + Tutorial)
25-September-2020	Dr. Jay Chakraborty (IL-5)	Dr. Kaushik Chakraborty (IL-6 + Tutorial)
26-September-2020	Dr. Sourab Sinha (Tutorial)	Dr. Rajeev R (IL-7 + 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: 20<sup>th</sup> 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:

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