



OUR PATRON

Prof. K. Umamaheshwar Rao
Director, NIT Rourkela

CHAIRMAN

Prof. Priyabrat Dash
HOD, Dept of Chemistry

COORDINATORS

Dr. Madhurima Jana
Dr. Bimalendu Adhikari

OVERVIEW / OBJECTIVES

The synthesis and modeling of (macro)molecules have evolved into mutually reinforcing disciplines, with the progress of cutting-edge research. These techniques are no longer confined to the advanced research landscape, now integrated into undergraduate curricula. This 5-day workshop aims to provide essential information and understanding to UG and PG students, as well as young researchers and faculty members on the fundamentals of the techniques of modeling and synthesis of molecules to macromolecules, including supramolecular polymers with biological and material significance. The key objective is the understanding of the methods towards the applications of these molecules/macromolecules across diverse scientific domains in chemistry, biochemistry, physics, and materials sciences.

PROGRAM / CONTENT :

Electronic structure theory-based molecular modeling

Molecular simulations: Atomistic & coarse-grained for biomolecules/macromolecules/polymers

Molecular modeling using machine learning and artificial intelligence

Synthesis, and applications of various covalent polymers, supramolecular polymers, and biomolecular assemblies including peptides

Characterization of macromolecules through various analytical and spectroscopic methods, including HPLC, GPC, CV, mass spectrometry, NMR spectroscopy, and UV spectroscopy

One-day visit of the student participants at NIT Rourkela campus

Hands-on sessions on instrumentation and modeling



Speakers

Prof. E D Jemmis
Dept. of Inorganic and Physical Chemistry
IISc Bangalore

Dr. Chanchal Chakraborty
Department of Chemistry
BITS Pilani, Hyderabad
Campus

Prof. Deva Priyakumar
CCNSB
IIIT Hyderabad

Dr. Dibyendu Das
Department of Chemical
Sciences
IISER Kolkata

Dr. Gokarneswar Sahoo
Dept. of Chemistry
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Dr. Padmabati Mondal
Department of Chemistry
IISER Tirupati



Dr. Rajat Kumar Das
Materials Science Centre
IIT Kharagpur

Dr R. S. Swathi
School of Chemistry
IISER Trivandrum

Dr Rajeev R
Department of Chemistry
NIT Rourkela

Dr. Suman chakrabarty
Department of Chemical and
Biological Sciences
SNBNCBS, Kolkata

Dr. Venkata Rao Kotagiri
Department of Chemistry
IIT Hyderabad

Registration link:

<https://shorturl.at/isGR3>

Workshop duration

25-September-2023 to 29-September-2023