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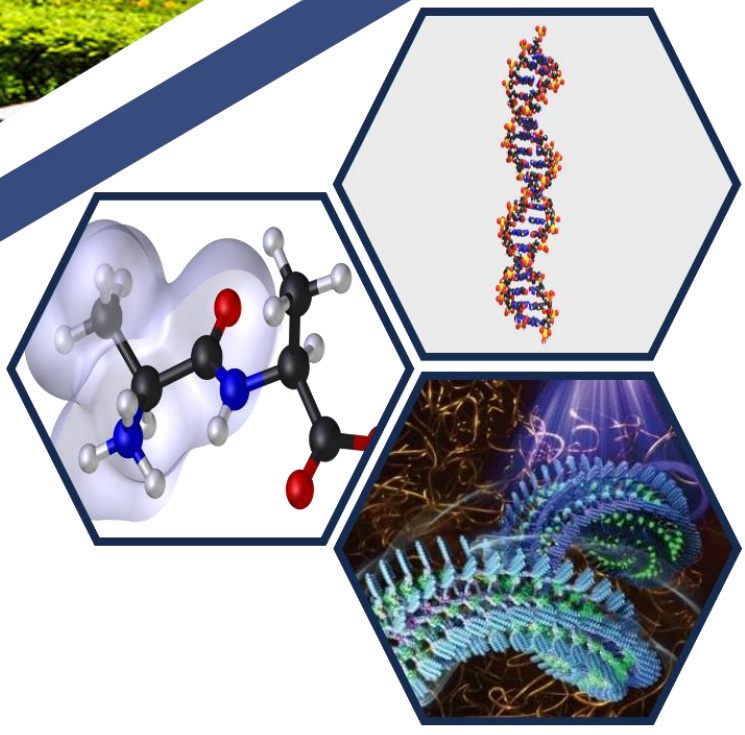


WORKSHOP ON

MODELING AND SYNTHESIS: MOLECULES TO MACROMOLECULES

2023

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 Hydrabad

Dr. Dibyendu Das
Department of Chemical Sciences
IISER Kolkata

Dr. Gokarneswar Sahoo
Dept. of Chemistry
NIT Rourkela

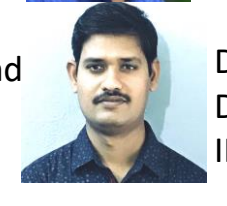
Dr. Padmabati Mondal
Department of Chemistry
IISER Tirupati

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 Hydrabad

Registration link:
https://shorturl.at/isGR3
Workshop duration
25-September-2023 to 29-September-2023

TENTATIVE BRIEF SCHEDULE

Date	3:30 PM - 6:30 PM	
Day-1 25-September-2023	• Inauguration • Keynote speech : Prof. E. D. Jemmis	
Day-2 to Day-5	**First Session (11:00 AM – 2:00 PM)** **Invited Lectures/Tutorials/Discussion**	**Second Session (3:30 PM – 6:30 PM)** **Invited Lectures/Tutorials/Discussion**
26-September-2023	Dr. Suman Chakraborty Dr. Chanchal Chakraborty	Dr. Venkata Rao Kotagiri Dr. R. S. Swathi
27-September-2023	Prof. Deva Priyakumar Dr. Gokarneswar Sahoo	Dr. Rajat Das Dr. Dibyendu Das
28-September-2023	Dr. Rajat Das Dr. Padmabati Mondal	Dr. Rajeev R Dr. Bimalendu Adhikari
29-September-2023	• Visit of the student participants to NIT Rourkela Campus • Distribution of Certificates & Valedictory Session	

TARGET PARTICIPANTS

Undergraduate, Post-Graduate Students in Science and Engineering, Research scholars, Faculties of Engineering and Science Colleges interested in teaching Supramolecular and Macromolecular Chemistry, Computational Chemistry, Computational Physics and Biology. Number of participants is limited to 100.

CERTIFICATE:

Certificates/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: 21st September, 2023. Registration LINK:** https://shorturl.at/isGR3

Venue: Department of Chemistry, NIT Rourkela, Hybrid mode. For online talks, **Meeting link will be shared to the registered participants**.

WORKSHOP COORDINATORS & CONTACT DETAILS:

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