Registration form

Name: _____

Designation : _____

Organization: _____

Address for Correspondence: _____

_____

_____

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E-mail:

Phone:

Particulars of Registration Fee:

DD/Transaction id: Date:

Amount: Bank:

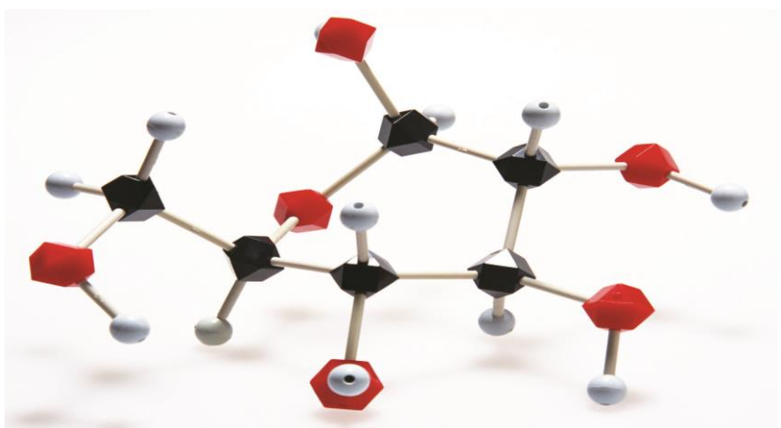
Branch:

Account Details

A/C No: 10138951784
IFS Code: SBIN0002109
A/C Name: CONTINUING EDUCATION NIT ROURKELA
Branch: State Bank of India, NIT Campus, Rourkela

Link for registration:

https://docs.google.com/forms/d/e/1FAIpQLScjYle4wasAeLgA8ayosaKB1HhUXbj8taAavIjtNzYrHX0l4g/viewform?usp=sf_link

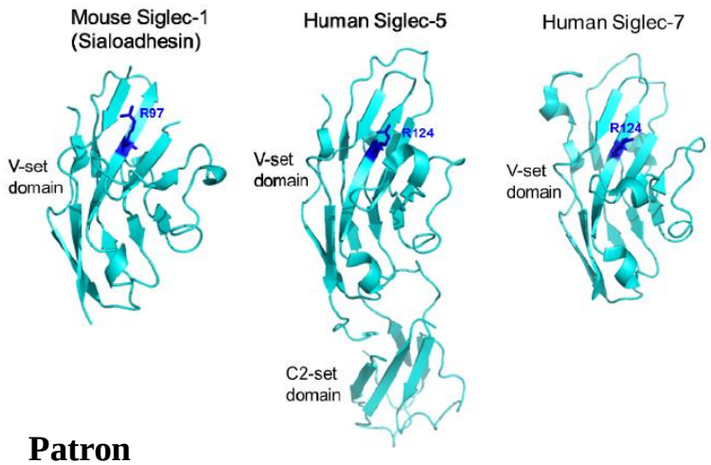


Molecular Structure

Course Venue

NIT Rourkela

NIT Rourkela is one of the premier national level institutions for technical education in the country and is funded by the Government of India. The main objective of the Institute is to produce quality Engineers and Scientists in Graduate and Post-Graduate levels in various branches of Engineering and Science. There are various research and development projects funded by different national and international agencies is in process at institute.



Patron
Prof. K. Umamaheswar Rao
Director, NIT Rourkela

Chairperson
Prof. Abanti Sahoo
HOD, Chemical Engg. , NIT Rourkela

Contact Details

Dr. Chandan K. Das
Coordinator
Assistant Professor,
Dept. of Chemical Engg.
NIT Rourkela, Rourkela, India
Mobile: 8132852063
Email : dasck@nitrkl.ac.in

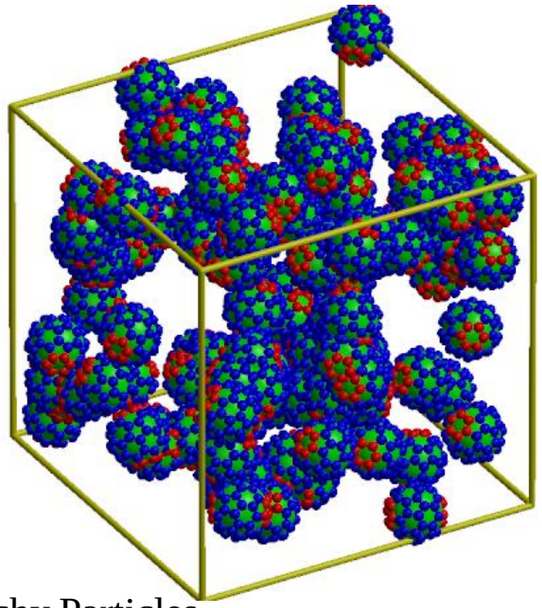
Online Short Term Course On Understanding of Molecular Simulation(UMS- 2023)

June 19 – 23, 2023

Organised by
Dept. of Chemical Engineering
National Institute of Technology Rourkela
Rourkela -769008
Odisha, India

Important Dates

Registration Deadline	16th June 2023
Confirmation to Participants through Email	17th June 2023
Commencement of Course	19th June 2023 (Online through Google Meet)

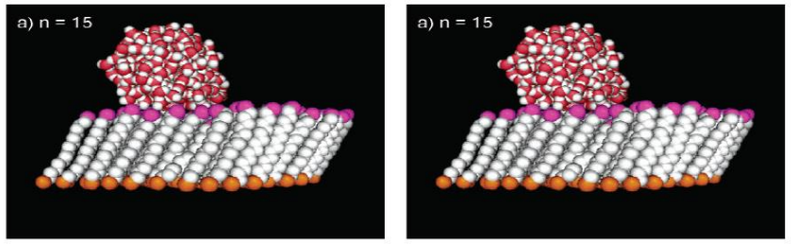


Patchy Particles

Introduction to the course

In this course, we will cover the basics of molecular simulation methods, and provide an overview of modeling tools for different problems of interest in science and engineering. The course is geared toward participants with an interest in molecular modeling, with or without prior experience in the area. At the end of this course, participants should have a general knowledge of the current state-of-the-art in molecular simulation, and be able to design and run simulations of systems of interest

The broad objective of the course is to provide understanding of methods, techniques, tools for modelling, simulation and performance analysis of engineering systems to resolve critical issues in real world environment.



Course Outlines

- Day-1
  - Elementary classical statistical mechanics, ensembles and fluctuations , thermodynamic connection, Partition function
  - Hands on Session: Simulations Tools
- Day-2
  - Monte-carlo Simulation: structure of a simulation program, periodic boundaries, generating initial configuration and velocities, property measurement, Markov chain, transition-probability matrix, detailed balance, Metropolis algorithm,
  - Hands on Session: Avogadro, PACKMOL, VMD
- Day-3
  - Molecular Dynamics: Initialization, the force calculation, integrating the equation of motion, integration algorithms, velocity Verlet algorithm
  - Hands on Session: LAMMPS
- Day-4
  - Free energy calculations methods: thermodynamic integration, pseudo-supercritical method, particle insertion method, free-energy perturbation, Gibbs-Duhem Integration
  - Hands on Session: Script file
- Day-5
  - Estimation of pressure, melting temperature, chemical potential, radial distribution function, auto-correlation function, diffusion coefficient
  - Hands on Session: GROMACS

Who should attend ?

- Person of Indian Origin
- Min. Qualification should be Post Graduate (Science) or B.Tech.(Technology)
- Professor /Scientist / Post-Doctoral Fellows / PhD Fellow / Industry person who are actively involved in R&D

The successful participants who will attend the whole will be given participation certificate.

Registration Type	Fees
Student	INR 200
Faculty Members	INR 500
Scientist from R&D Organization/Industry Person	INR 1000

The course fee includes online course material. Participants (Faculty members and students) from NITRKL are exempted from paying registration fees.

Resource Persons

Dr. Atanu Kumar Metya
Assistant Professor,
Dept. of Chemical and Biochemical Engg.
IIT Patna, Patnar,India

Dr. Anand Bharti
Assistant Professor,
Dept. of Chemical Engg.
BIT Mesra, Ranchi, India

Dr. Chandan Kumar Das
Assistant Professor,
Dept. of Chemical Engg.
NIT Rourkela, Rourkela, India