Self sponsored three days workshop on

"Molecular Dynamics Simulation & Analysis"

5th August to 7th August 2022

Organized by

Department of Mechanical Engineering
Dr. B. R. Ambedkar National Institute of Technology
Jalandhar-144011 Punjab
www.nitj.ac.in

Course Co-ordinator

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Objective of the Course

Molecular modelling and simulation involve developing representations of physical systems at atomistic/molecular-level detail, and using such models to simulate (or mimic) physical processes/phenomena on a computer for studying properties of interest. Molecular simulations can also be used to calculate or predict properties and quantities that may be difficult to observe experimentally. The workshop will introduce the field of molecular modelling and simulation to the participants through lectures, demonstrations, and hands-on sessions. In particular, the focus will be on the classical molecular dynamics (MD) simulation technique. The simulations will be conducted and demonstrated using Materials Studio and the open-source software package LAMMPS. The software packages VMD and OVITO (also open source) will be used to visualize molecular models and simulation results.

This workshop aims to review various molecular simulation techniques with a focus on how practical industrial problems can be solved using molecular simulations by helping screen a range of potential raw materials without the need to actually synthesise such products/chemicals. Such simulation techniques may reduce the huge amount of money spent on chemicals and human resources, for synthesizing specific products. The workshop shall involve experts working in the area of molecular simulations who are engaged in using such techniques for developing their own codes or are using similar software to understand and solve fundamental and practical problems related to Mechanical Engineering.

Registration

The registration fees for attending the Workshop:

From NIT Jalandhar : INR 1000/-

Outside NIT Jalandhar: INR 1200/-

Details for Payment:
A/C name: NITJ CCE
A/C no.: 50100324249116
IFSC code: HDFC0000046

Please register online on or before 31st July2022. Seats are limited therefore applications will be considered on a first-come, first-served basis (date of receipt of registration). Preference will be given to faculty members, and people from the industry. The maximum number of participants allowed for this course will be 100. You are requested to mail the registration slip with complete information to md2022@nitj.ac.in.

Who can apply:

This course is open to faculty members from Engineering Institutes/ Colleges/ Polytechnics and practising Engineers and Researchers from Industries and R&D institutions.

General Instruction:

Participants are requested to have Laptops for a better learning experience during practice sessions on LAMMPS, MATERIALs STUDIO, VMD, NANOENGINEER, and OVITO Software.

Highlights of the Course:

Day1:

- Introduction to Molecular Dynamics & its application.
- Guidelines how to install LAMMPS,OVITO,VMD,Nano-Engineer.

Day 2:

- Introduction to Materials Studio
- Introduction to LAMMPS

Day 3:

- Hands-on practice

Chief Patron

Sh. Subhash Chandra Ralhan
Chairperson, BOG,
Dr. B R Ambedkar National Institute of Technology , Jalandhar

Patron

Professor Binod Kumar Kanaujia
Director, Dr. B R Ambedkar National Institute of Technology, Jalandhar

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Dr. Pramod Kumar
HOD, Department of Mechanical Engineering, Dr. B. R. Ambedkar National Institute of Technology, Jalandhar

Departmental Organizing Committee

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Student Volunteer

Mr. Pramod Rakt Patel
Ms. Deepa Bedi

About NIT-Jalandhar

The Institute is named after Bharat Ratan Dr B. R. Ambedkar, founder of Indian Constitution. The institute came into existence in the year 1988 as Regional Engineering College on a beautiful campus of about 154 acres close to the heart of Jalandhar city. The institute obtained the status "Institute of National Importance" by Act of Parliament in 2007. The institute is located on the G.T Road Amritsar bye-pass at a distance of 15 km from Jalandhar Bus Stand, 12 km from Jalandhar City Railway Station, and 18 km from Jalandhar Cantt. railway station. The institute is well connected to the National Capital through rail and road link. The institute is ranked 49 in the NIRF ranking 2021 and THE world ranking of 800-1000.

About ME Department

The Department of Mechanical engineering was founded in 1990 and has grown as one of the dynamic departments of the Institute over the last three decades. The department offers B Tech, M Tech (Design & Thermal) and PhD programmes. The B.Tech program is accredited by the NBA. At presently (61) sixty one research scholars are registered in the department for pursuing Ph.D.