SELF SPONSORED

2-WEEK SHORT TERM TRAINING PROGRAM

ON

Molecular Modelling and Molecular Dynamics Simulations for Functional Nanomaterials and Nanocomposites

June 30- July 12, 2025

(Hybrid Mode)

Convener

Dr. Mithilesh K. Diksiht Dr. Kumar Abhishek Dr. Ganesh Iyer





by:

Department of Mechanical and Aerospace Engineering Institute of Infrastructure, Technology, Research and Management, Ahmedabad, India

ORGANIZING COMMITTEE

PATRON

Prof. P.K. Jain Director General, IITRAM

CHAIRMAN

Prof. M.K. Barua Director, IITRAM

Dr. Dileep K. Gupta HOD, Department of Mechanical and Aerospace Engineering, IITRAM

CONVENER

Dr. Mithilesh K. Diksiht Dr. Kumar Abhishek Dr. Ganesh Iyer Department of Mechanical and Aerospace Engineering, IITRAM

IMPORTANT DATES

- Start of Registration: April 05, 2025
- Last Date of Registration: June 20, 2025
- STTP Dates: June 30 July 12, 2025
- Registration Link: <u>https://forms.gle/d7rWuCTwnQyDWBRA7</u>

Registration Fee

- Students (UG/PG/Ph.D) Rs. 1770.00
- Faculty/Industry/Scientist/R&D 2360.00
- Group Registration 1 registration free on group of 3 participants from same affiliation.

ABOUT IITRAM

The Institute of Infrastructure Technology Research And Management (IITRAM) has been established by the Government of Gujarat as an Autonomous University and has been mandated to bring about significant change in Engineering Education with respect to Technical and Managerial knowledge in the area of Infrastructure. IITRAM has been established to contribute to the community of world-leading researchers by promoting excellence within disciplines and inter-disciplinary teams, tackling global challenges, providing cultural enrichment and thereby, benefitting the economy. With a continuously updated curriculum, the University strives to achieve excellence in teaching and research, with a vision to be amongst the best institutions in our country and abroad. One of the aims of the University is to provide a conducive environment that fosters multi-front skill development and overall growth of the students.

ABOUT DEPARTMENT

The Department of Mechanical Engineering at IITRAM, Ahmedabad started after one year of the inception of university in 2014 and has been offering B.Tech Mechanical Engineering, M. Tech. Mechanical (Industrial Infrastructure) and Doctoral Programs. The Department of Mechanical Engineering was renamed as Department of Mechanical and Aerospace Engineering by incorporating Aerospace Engineering in 2020. The students of all tiers have access to both expert faculty members in the department and institute supported industry engagement opportunities. The department has extensive laboratory and infrastructural facilities for teaching, training, research and development.

ABOUT STTP

This STTP aims to provide participants with in-depth knowledge and hands-on experience in Molecular Modelling and Molecular Dynamics (MD) Simulations, focusing on their applications in engineering and materials science. The program will cover fundamental concepts, advanced simulation techniques, and their real-world implementation in the study of functional nanomaterials and nanocomposites.

The training program is specially designed for a diverse group of participants, including faculty members, researchers, scientists, postgraduate and Ph.D. students, as well as final-year undergraduate students who are keen to enhance their understanding and skills in this domain. Through expert lectures, practical sessions, and interactive discussions, participants will gain insights into the role of MD simulations in predicting material properties, optimizing material performance, and designing novel nanocomposites for engineering applications.

OBJECTIVES

This Short-Term Training Program (STTP) aims to train faculty, researchers, and postgraduate students, and to facilitate knowledge exchange in *Molecular Modelling and Molecular Dynamics simulations*. The program includes expert lectures from premier institutes like NITs, IITs, and leading industries, promoting interdisciplinary collaboration and research partnerships across academia and industry.

TOPICS

- Introduction to MD Simulations
- Statistical Mechanics and Statistical Averaging
- Statistical Ensemble
- Macroscopic Parameters
- Temperature Scaling
- Pressure Scaling
- Inter-Atomic Potentials
- Numerical Time Integration Techniques
- Atomistic & Molecular Modelling in Material Studio
- Setting Up Nanocomposite Simulations
- Running MD Simulations in Material Studio
- Post-processing & Visualization of Results
- Case Study & Hands-on Practice
- Running MD Simulations in LAMMPS
- Reactive MD & Force Field Selection
- Mechanical Property Simulations
- Thermal & Transport Properties
- Interfacial Interactions in Nanocomposites
- Machine Learning & MD Simulations
- Research Applications & Future Directions

ELIGIBILITY

This program is interdisciplinary in nature, making it open to faculty members, research scholars, and finalyear UG and PG students from all branches of engineering, as well as from mathematics, physics, and chemistry. Scientists from R&D organizations and professionals from industry are also eligible to participate in this STTP.

SELECTION

Seats are limited to 30 and will be allotted on a firstcome, first-served basis. Selected participants will be notified via email. Certificates will be given only upon full attendance.

BANK DETAILS

The non-refundable registration fees should be paid only by ONLINE TRANSFER in account of:

Bank Name: Axis Bank Ltd Bank Account Name: Institute of Infrastructure Technology Research and Management Bank Account Number: 923010019592531 IFSC Code: UTIB0002645 Branch Name: Hatkeshwar Branch, Ahmedabad Micr Code: 380211048 Branch Address: Khokhra Circle, Maninagar (East) Ahmedabad – 380026.

Note: Please mention 'STTP MD-2025' in the description/remark during payment and attach payment proof while registering through the Form. After Submission of fees the registration can be done using the following link:

Registration Link:

https://forms.gle/d7rWuCTwnQyDWBRA7

Accommodation may be provided on a paid basis at nominal charges.

CONTACT US

For more information you may contact to:

- Dr. Mithilesh K. Dikshit, IITRAM <u>mithileshdikshit@iitram.ac.in</u> Mob: +91-8247095848
- Dr. Ganesh Iyer, IITRAM <u>ganeshiyer@iitram.ac.in</u> Mob: +91 73766 66176
- Dr. Kumar Abhishek <u>kumarabhishek@iitram.ac.in</u> Mob: +91 87636 55384