

About the Institute

Maulana Azad National Institute of Technology Bhopal (MANIT), an Institute of National Importance, is formerly known as Maulana Azad College of Technology (MACT).

Institute is named after the great scholar and 1st Education Minister of Govt. of India, Maulana Abul Kalam Azad. The Govt. of India and Govt. of Madhya Pradesh jointly sponsored the Institute in 1960 to attract bright young engineering students across the country. Institute is successfully producing highest quality skilled manpower to cope up with challenges of modern technological advances with more than 250 faculties and 6000 students. The Institute offers 09 UG and 30 PG courses and also Ph. D. research programmes. For details about the institute please visit us at <https://www.manit.ac.in/>



About the Department

Established in 2007, the Department of Chemical Engineering at MANIT Bhopal is dedicated to excellence in teaching, research, and innovation. The department offers undergraduate, postgraduate, and doctoral programmes with a strong emphasis on quality education and interdisciplinary research. Equipped with modern laboratories and advanced research facilities, the department actively promotes academic excellence through workshops, training programmes, conferences, and collaborations with academia and industry.

Course Overview

This 5-day Faculty Development Programme (FDP) provides a comprehensive introduction to modern computational techniques for solving challenges in chemical, materials, and energy engineering. The programme integrates Molecular Dynamics (MD), Density Functional Theory (DFT), Periodic DFT, Monte Carlo simulations, and photovoltaic device modeling to bridge theoretical concepts with practical research applications.

Participants will gain hands-on experience with state-of-the-art computational tools, including **NAMD**, **GROMACS**, **Gaussian**, **Quantum ESPRESSO**, **Towhee**, and **SCAPS-1D**, while exploring applications in carbon capture, catalyst design, molecular interactions, micropollutant separation, adsorption, phase equilibria, advanced materials, metal-organic frameworks (MOFs), semiconductors, and photovoltaic devices.

Through a combination of expert lectures, practical demonstrations, and guided computational exercises, the programme will enable participants to develop molecular models, perform atomistic and electronic structure simulations, predict thermodynamic and transport properties, and investigate materials for sustainable energy and environmental applications. The FDP aims to equip participants with the computational skills required to address contemporary research problems and accelerate innovation in academia and industry.



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Faculty Development Programme (Online mode)

on

Advanced Computational Methods for Chemical, Materials and Energy Applications- (ACCME 2026)

August 21st – 25th, 2026



Patron

Prof. Karunesh Kumar Shukla
Hon'ble Director,
MANIT, Bhopal

Chairman

Dr. Sunder Lal Pal
Associate Professor & HOD
Department of Chemical Engineering
MANIT Bhopal

Coordinators

Dr. Nabendu Paul
Dr. Rupak Kishor
Dr. Subhajit Patra
Dr. Sunder Lal Pal

Organised by

Department of Chemical Engineering,
Maulana Azad National Institute of
Technology Bhopal
Pin: 462003, Madhya Pradesh, India

Course Objectives

- Introduce modern computational methods for chemical, materials, and energy applications.
- Develop a foundation in MD, DFT, Periodic DFT, Monte Carlo simulations, and semiconductor device modeling.
- Enhance understanding of computational approaches for sustainable engineering solutions.
- Provide hands-on training using NAMD, GROMACS, Gaussian, Quantum ESPRESSO, Towhee, and SCAPS-1D.

Important Dates

Registration Deadline	17 th August 2026
Confirmation to Participants through Email	18 th August 2026
Commencement of Course	21 st August 2026 (Online)

Resource Persons

- Dr. Tamal Banerjee (IIT Guwahati)
- Dr. Debashis Kundu (ICT Mumbai)
- Dr. Anand Bharti (BIT Mesra)
- Dr. Nikhil Khatavkar (MANIT Bhopal)
- Dr. Rupam Sinha (NIT Trichy)
- Dr. Papu Kumar Naik (Patliputra Univ.)
- Dr. Nabendu Paul (MANIT Bhopal)
- Dr. Rupak Kishor (MANIT Bhopal)
- Dr. Dharendra Kumar Mishra (Lawrence Berkeley National Laboratory, USA)

E-certificates will be provided to participants who successfully complete the course.

Day-1

- *Theory: Introduction to Density Functional Theory (DFT) & Molecular Dynamics for chemical, materials & energy applications.*
- *Key Learning : Geometry optimization, electronic structure, and reaction energetics using GAUSSIAN for carbon capture and separation processes.*

Day-2

- *Theory: Advanced Molecular Dynamics Simulations in separation and energy systems.*
- *Key Learning : Fundamentals of MD, simulation workflow, force fields, Trajectory analysis for micropollutant separation, and biomolecular interaction; Application of MD Simulation and AI in modelling of Electrolytes for energy storage device.*

Day-3

- *Theory: Monte Carlo Simulations for Complex Chemical Systems*
- *Key Learning : Phase equilibrium, adsorption, and thermophysical property prediction using TOWHEE.*

Day-4

- *Theory: Periodic Density Functional Theory for materials and energy applications*
- *Key Learning : Materials modeling using Quantum ESPRESSO for semiconductor materials, catalysts, and batteries.*

Day-5

- *Theory: Photovoltaic Device Modeling*
- *Key Learning : Photovoltaic device simulation and performance optimization using SCAPS-1D.*

Registration Form

Name:
Designation :
Organization:
Address for Correspondence:
E-mail:
Phone:
Particulars of Registration Fee
DD/Transaction ID:
Date: Amount:
Bank: Branch:

Link for online registration:

<https://forms.gle/fyBztu85WGYnuX6z6>

Registration Type	Fees (incl. GST)
Student	INR 500
Faculty Members	INR 750
Scientist from R&D	INR 1500
Organization/Industry/ Others	

Bank Account Details

Beneficiary name: Director, MANIT Bhopal
Branch name: SBI, MANIT Branch
Account number: 10020150107
IFSC code: SBIN0001608

Participants from MANIT Bhopal are exempted from paying registration fees.

Address for Communication

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