Online short-term course on

Basic principles of "DFT Calculations & Molecular Dynamics Simulations"

(23rd to 27th November, 2020)

(Sponsored by TEQIP-III)

Organized by

Department of Chemical Engineering,
Malaviya National Institute of Technology
Jaipur-302017

Organizing committee

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(Director, MNIT Jaipur)

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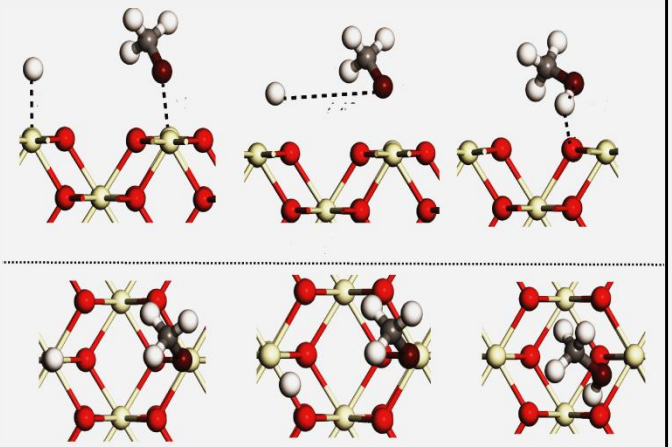


About MNIT

The Institute, earlier known as MREC, was established in 1963 as a joint venture of the state and central governments. Later in 2002, the college was given the status of National Institute of Technology. MNIT campus spreads over 325 acres of lush green area in the prime location of Jaipur city. The institute offers various academic activities in addition to research, consultancy and development. The Institute offers UG and PG (M. Tech./M.Sc. & Ph.D.) level courses to about 5000 students in almost all leading fields of engineering, technology, management, and sciences. MNIT Jaipur ranked at 35th position in NIRF 2020 Ranking.

About the Department

The Department of Chemical Engineering was commenced in the year 1988. The PG programmes of M.Tech. and Ph.D. in chemical engineering was started in year 2006 and 2004, respectively. The current sanctioned strength of B.Tech. and M.Tech program is 96 and 30, respectively. The department is well equipped with good undergraduate and research laboratories. The curriculum has been designed to meet the programme goals and objectives that lay more stress on learning under the guidance of a vibrant and highly qualified faculty.

About the Short Term Course

Density functional theory (DFT) is an extremely successful approach of molecular modeling, for the description of the ground state properties of chemical and biological species, while molecular dynamics (MD) simulation technique helps us to visualize the exact trajectory at molecular level and helps us in predicting macroscopic properties of the system based on microscopic observations.

The objective of this course is to learn the fundamental concepts of *ab-initio* calculations (DFT) and MD simulation. Both the techniques have a wide range of applications in various disciplines of engineering sciences. The STC will focus on the basic principles and applications of these computational techniques through intensive lectures, hands on sessions and interesting case studies.

Key topics covered in STC

- Basic fundamentals of DFT calculations
- Rate calculation of chemical and biological reactions using transition state theory.
- DFT calculation in chemical catalysis: CO_2 reduction and ammonia synthesis
- Ab-initio micro-kinetic modeling and simulations
- Development of force-field parameters for coarse-grain modeling
- Conformational analysis and binding free energy perspectives from MD simulations
- Applications and Interesting case studies based on the techniques.
- Hands on experience of BIOVIA Materials Studio and GROMACS simulation package.

Key Speakers

Prof M. Ali Haider
Associate Professor,
Department of Chemical Engineering,
IIT-Delhi

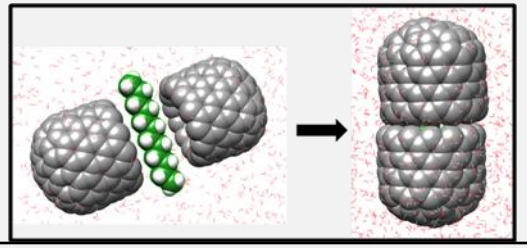
Dr. Piyush P. Wanjari
Assistant Professor,
Department of Chemical Engineering,
VNIT, Nagpur

Dr. Ritwik K.
Application Scientist,
Dassualt systems, Bengaluru

Dr. Shelaka Gupta
Assistant Professor,
Department of Chemical Engineering,
IIT-Hyderabad

Dr. Uzma Anjum
Research Fellow, Department of Chemical and Bio-molecular Engineering, NUS Singapore

Dr. Inderdip Shere
Research Associate,
Department of Chemical Engineering,
IIT-Bombay



Registration Process

- Registration is open to faculty members, industrial personnel, PDF, RA, Ph.D., PG and UG students. Limited seats, shortlisting criteria: first come first serve basis.
- The participants will be awarded with an ***e-certificate*** based on successful completion of the course
- Please click on the link below for registration.
- Last date of registration is **15th November 2020**

Link for Registration

Registration Fees:

The participation fee including GST is mentioned below.

For MNIT Students (UG/PG/PhD):	Rs. 250
Other Institute Student (UG/PG/PhD):	Rs. 500
People from Academics/Industry:	Rs. 750

Payment mode: NEFT/IMPS

Account Details:

Registrar, MNIT Jaipur (TEQIP-III)

A/C No. 36875887782, SBI, MNIT Campus Jaipur,

IFSC Code: SBIN0015921

Contacts for registration / support

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