

ABOUT NIT UTTARAKHAND

National Institute of Technology, Uttarakhand is amongst the emerging NITs, located in Srinagar Garhwal. It was established in 2009 under the Act of Parliament of India by the Ministry of Human Resource Development and designated with the status of "Institute of National Importance". The temporary campus of NIT Uttarakhand is functional from two campuses i.e. Polytechnic and ITI. Recently NIT-UK has started its operations from a Satellite campus at MNIT Jaipur for the B.Tech. students. The Institute offers B.Tech., M.Tech. in Engineering branches and Ph.D. courses in Engineering and Science disciplines. TEQIP-III programs is running in the Institute since April 2018. With continuous efforts to create research oriented environment, Department of Chemistry, NIT Uttarakhand is offering a workshop on "DENSITY FUNCTIONAL THEORY AND ITS APPLICATIONS USING GAUSSIAN SOFTWARE".

ABOUT MNIT JAIPUR

Malaviya National Institute of Technology is one of the premier NITs of India, fully funded by Ministry of Human Resource Development (MHRD), Government of India. The institute was given the status of a National Institute of Technology and Deemed University on June 26, 2002, and proclaimed the Institute of National Importance through Act of Parliament on August 15, 2007. The Institute offers undergraduate and post graduate (B. Tech., B.Arch., M. Tech., M. Plan., M.Sc., MBA and PhD) programmes to about 5000 students in leading field of Engineering, Technology, Architecture, Management and Sciences. The institute is actively engaged in research, consultancy and developmental activities, besides imparting regular teaching.

ABOUT SLIET LONGOWAL

Sant Longowal Institute of Engineering & Technology (SLIET), Longowal, established by the Government of India, provides technical education in emerging areas of Engineering & Technology. The institute was set up in 1989 and is fully funded by Ministry of Human Resource Development, Government of India. The Institute offers programmes at Certificate, Diploma, Degree, Post-graduate (M.Tech., M.B.A. and M.Sc.) and Ph.D. levels in Engineering and Technology, Science, Humanities, Management.

PATRONS

Prof. Shyam Lal Soni,
Director, NIT Uttarakhand

&

Prof. Udaykumar R Yaragatti,
Director, MNIT Jaipur

&

Dr. Shailendra Kumar Jain
Director, SLIET Longowal

CONVENERS

Dr. Pankaj Kandwal
(NIT Uttarakhand)

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(MNIT Jaipur)

Dr. Damanjit Singh
(SLIET Longowal)

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ADVISORY COMMITTEE

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Dean Academics

Dr. Vinod Singh Yadav
Coordinator TEQIP-III

VENUE

VLTC building, MNIT Jaipur
J.L.N. Marg, Jaipur

CONTACT PERSONS

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TEQIP-III

(under Twinning Activity)

Sponsored

ONE WEEK TRAINING WORKSHOP

on

DENSITY FUNCTIONAL THEORY AND ITS APPLICATIONS USING GAUSSIAN SOFTWARE

24th – 28th February 2020

Jointly Organized by



Department of Chemistry,
National Institute of Technology, Uttarakhand
Satellite Campus, MNIT Jaipur-302017

&

Department of Chemistry,
Malaviya National Institute of Technology Jaipur
J.L.N. Marg, Jaipur-302017

&

Department of Chemistry,
Sant Longowal Institute of Engineering and Technology
Longowal-148106

ABOUT THE TRAINING WORKSHOP

Density Functional Theory (DFT) has been used worldwide for geometry optimization, energy minimization, property calculations, spectroscopic parameter calculations, etc. in all branches of Chemistry. This workshop will introduce the underlying principles of DFT and familiarize the participants with the insights of the laws (and impart knowledge on new approaches in DFT). The program will also be very beneficial and important for Faculty members, Research Scholar and Masters Students who are working in the area of DFT theory and Computational Chemistry. The experienced speakers will provide the platform to the participants to interact, to share the knowledge and solve the difficulties faced. In this way, this will be unique of its own kind, where the beginners as well as trained participants can grab ample chance to learn new approaches in DFT.

TOPICS TO BE COVERED IN WORKSHOP

This training workshop will cover following topics (but not limited to)-

- ❖ Introduction to DFT and its capabilities
- ❖ Applications in Chemistry
- ❖ Hands-on practise on GAUSSIAN software
- ❖ Chemical property calculation on molecules
- ❖ Input file preparation and output data analysis
- ❖ Future prospects

SPEAKERS

Expert members from Research Institutes/ BARC/IITs/NITs/reputed organizations/labs will give insights on various topics and themes of the workshop.

WHO SHOULD ATTEND THE WORKSHOP

The Masters/Ph.D. students, faculty members, research scientists working in the area of Computational chemistry are welcome to attend the training program. Candidates who are interested to learn the basics and know-how of the topics in density functional theory (DFT) can also participate and extend their domain of knowledge.

REGISTRATION

The detail of the registration fee is given in the following table:

Delegates	Fees
Industry Persons	4000/-
Faculty and Engineers	2000/-
Students	500/-

- Registration fee (non-refundable) includes registration kit, course certificate, tea and lunch.
- No TA/DA will be provided to the participants.
- No registration fee for participants from TEQIP-III funded Institutions.

MODE OF PAYMENT

The registration fee should be paid online and the filled-in registration form counter signed by the Supervisor/Head/Principal of the concerned Institute/organization/university must be sent at **workshop.dft@gmail.com** on or before 20th February 2020. For online payment, details of NIT Uttarakhand Bank account are given below:

A/C Name	NIT Uttarakhand
Bank Name	SBI, Srinagar-Garhwal
A/C No.	37843015175
IFSC Code	SBIN0003181

ACCOMMODATION

Accommodation will be provided in the Guest House/Hostels of MNIT Jaipur as per the availability and on payment basis.

HOW TO REACH

Workshop will be conducted at NITUK Satellite Campus, VLTC building, MNIT Jaipur. The campus is well connected by Air, Rail, and bus transport. For any further query, please write to:
workshop.dft@gmail.com

REGISTRATION FORM

TEQIP-III

(under Twinning Activity)

One Week Training Workshop
on

DENSITY FUNCTIONAL THEORY AND ITS APPLICATIONS

USING GAUSSIAN SOFTWARE

(24th – 28th February 2020)

Name: _____

Designation & Official Address: _____

Highest Academic Qualification: _____

Accommodation Required: Yes/No

Registration Fee Details: _____

(Category: Faculty/students/industry person/)

Institute under TEQIP-III (Yes/No): _____

Payment mode: Online/Cash

Transaction ID: _____

Bank Name: _____ Amount: _____

Address for Correspondence: _____

_____ Pin: _____

Mobile: _____ Email: _____

Signature of Applicant: _____

Authorized Signatory with Seal

(Registration form counter signed by the Supervisor/Head/Principal and Fee should be submitted online along with receipt of payment on or before 20th February 2020. Registration may be accepted at the registration counter provided seats are available.)