



NATIONAL INSTITUTE OF TECHNOLOGY
WARANGAL

Warangal - 506 004, Telangana

TEACHING LEARNING CENTRE

(A Pandit Madan Mohan Malaviya National Mission on Teachers and Teaching)



*A Six-Day Online Faculty Development
Programme with hands on experience on*

APPLICATIONS OF DFT

(DENSITY FUNCTIONAL THEORY) IN

**TEACHING AND LEARNING CHEMISTRY, PHYSICS
& MATERIAL SCIENCE - WITH SOFTWARE FOR
CHEMISTRY AND MATERIALS (SCM-AMS)**

19th -24th March 2021

Call for Registration and Participation

Coordinators

Dr. M. Raghasudha, *Department of Chemistry*

Dr. Ravinder Pawar, *Department of Chemistry*

Prof. A. Ramachandraiah, *Coordinator, TLC*

Organized by the

DEPARTMENT OF CHEMISTRY

In Association with the

TEACHING LEARNING CENTRE

*Established under the Scheme of PMMMNMTT,
Ministry of Education, Govt. of India*



Overview of the FDP:

The role of density function theory (DFT) to probe the geometries, energy minimization, property calculations, spectroscopic parameter calculations, etc proven to be enormous. Therefore, understanding the theory and its applications have received widespread attention. This FDP consists of two parts where the theory associated with the DFT, and various aspects of Chemistry, Physics and Materials will be dealt. The second part will be hands on experience with SCM-AMS software where the application of DFT to various challenging problems faced by Chemists, Physicists and Materialist will be demonstrated with the help of SCM-AMS. Further, participants will be remotely provided with computer and SCM-AMS software for hands on experience to practice and workout various problems of Chemistry, Physics and Materials.

This Faculty Development Workshop is aimed to impart basic principles and advanced knowledge related Computational Chemistry to faculty and researchers and to open new vistas for them in teaching. Further, this workshop provides a platform for interaction and exchange of ideas on current trends in the fields of Computational Chemistry with eminent people in the field.

Objectives of the FDP:

- To enable the participants to learn the Basic Principles of Density Functional Theory (DFT) and its applications to Chemistry, Physics and Material Science.
- To facilitate the participants to DFT based methods and protocols through hands-on experience with the help of SCM-AMS software.
- To probe the role of DFT to develop new molecules, materials and solve the problems faced by the experimentalists.
- To empower the participants to transfer their learning experiences into their classroom-teaching practices.

Topics to be covered:

- Basics of Quantum chemistry, Density functional theory and various aspects of Chemistry, Physics and Materials
- Applications of DFT with hands on experience includes:
 - a. Installation of various Softwares.
 - b. Building molecules and materials using Avogadro, Gabedit, SCM-AMS
 - c. Solving problems of organic, inorganic and physical chemistry
 - d. Understanding Solid State Physics and Material Science with the help of SCM-AMS

Resource Persons:

Eminent Faculty from abroad, IITs, NITs, Central Universities, Teaching Learning Centres and Senior Faculty from NIT Warangal.

Mode of Delivery:

Resource Persons will deliver the online lectures through Google-Meet platform and hands-on session will be conducted by providing remote access to the computers in NITW via Anydesk. The essence of the FDP is to improve the teaching ability of the teachers and enabling the learners to learn. The theme of the FDP is a way in building capacity of making better teachers. Lectures can be presentation mode, Discussions and hands-on sessions. Ultimate goal of the FDP is to develop the faculty members in the new pedagogy and emerging areas of science and technology.

Registration is open to:

The program is open to all NBA and AICTE approved Engineering/Polytechnic college teachers, Degree college lecturers, research scholars and P.G. students. The number of participants is approximately 100 and selection will be based on priority basis. The Brochure and details of the Registration Form can be downloaded from the institute website <http://www.nitw.ac.in>

How to Register:

Eligible candidates may apply by submitting the scanned copy of the filled registration form (attached with this mail/brochure) by E-mail to adft.tlcpms21@gmail.com on or before **17.3.2021** along with the requisite Registration Fee.

Registration Form:

Faculty members can also complete their Registration online by filling the following Google form

https://docs.google.com/forms/d/e/1FAIpQLSd8jGITkYf8_VoVHSd6MXqBNBVZS9-4bU41q8NPtHWlqGwBNQ/viewform?usp=sf_link

Note: Keep the payment receipt ready as a PDF file (size < 1 MB)

Registration Fee:

Category of Participants	Reg. Fee
Faculty Members	750/-
Research Scholars	400/-

Note: Registration Fee for Faculty and Students of SC/ST category is half of the amounts mentioned above as applicable.

Bank Details:

Registration Fee may be remitted through NEFT to the Bank account given below. Proof of remittance of the requisite registration fee (with transaction number if online transaction) shall be uploaded in the Google Form.

Account Name	Director, Research Account, NITW
Account Number	62266262236
Bank	State Bank of India (SBI)
Branch	NIT Warangal Campus
IFSC code	SBIN0020149

Confirmation of Participation:

On receipt of the Google Form and Fee Remittance Receipt, participants will be sent confirmation of their participation through email by **18.3.2021**. As the programme is conducted online with the number of participants in the workshop is limited to 100. Candidates are advised to register early to avoid disappointment.

Brief profile of the Department:

The Department of Chemistry was established in the Year, 1959, as an integral part of the Regional Engineering College Warangal (RECW). Since its inception, the department is greeted as one of the most academically active departments in the Institute. Department offers chemistry course to all engineering branches and two years M.Sc. Chemistry with specialization in Organic and Analytical Chemistry. The Department has been conducting cutting-edge research in contemporary topics of Organic, Inorganic, Physical and Analytical Chemistry. In the Department, various state-of-the-art facilities such as 400 MHz NMR, HRMS, gas chromatography, HPLC, FTIR, UV-Vis-NIR, fluorescence, electrochemical workstation, computational chemistry software, etc. are available. As a part of continuing education and outreach activities, Department organized several National and International Conferences, Seminars and Workshops.

Teaching Learning Centre of NIT Warangal:

The Teaching Learning Centre (TLC) has been established at NIT Warangal with grants from the MHRD, through its scheme "**Pandit Madan Mohan Malaviya National Mission on Teachers and Teaching (PMMMNMTT)**". Under this Scheme, a separate building has been built exclusively for the TLC activities, with the state-of-art training facilities that include a studio for production and uploading of video and e-lectures on various subjects of higher education, training halls to train the faculty in various theme areas of Science and Technology, humanities and social sciences, linguistics and communication skills, pedagogy and cognition evaluation, etc. among others. Many senior and young faculty are associated with this Centre as Core-Team. One of the important objectives of the Centre is to conduct training programmes for the aspiring, newly inducted and in-service faculty in science, engineering, social sciences disciplines in higher education. Other activities of the TLC include preparation of print and e-learning materials, offering on-line courses, curriculum design, carrying out research in educational technology and pedagogy and integrating with ICT into teaching-learning process. The TLC has special programmes of training for the marginalized and women-faculty.

About NIT Warangal:

National Institute of Technology Warangal, formerly known as Regional Engineering College was established in 1959. Over the years it has developed into a premier institute of higher learning and is ranked among the top technical education institutions in India. There are 14 Departments offering eight undergraduate and 31 post-graduate programs besides doctoral programmes. About 5000 students across the country and about 500 international students study on the campus. It is a fully residential campus sprawling over 250 acres with excellent infrastructure in the form of state of the art library, seminar halls, guest houses and research laboratories.

For any queries regarding the FDP, please contact the Programme Coordinators:

Name of the FDP Coordinator, Designation, Contact details, Email ID

Dr. M. Raghasudha, Asst. Prof., Department of Chemistry, 9550083100,

adft.tlcpms21@gmail.com

Dr. Ravinder Pawar, Asst. Prof., Department of Chemistry, 9490917338

adft.tlcpms21@gmail.com

For further details about Teaching Learning Centre, please contact:

Prof. A. Ramachandraiah

Professor-in-Charge and Coordinator,
Teaching Learning Centre (TLC), NIT Warangal
E-mail: archem@nitw.ac.in; mtlc.nitw@nitw.ac.in
Office: 0870-2462686.

PANDIT MADAN MOHAN MALAVIYA TEACHING LEARNING CENTRE

