

Directorate of Quality Assurance and Accreditation Internal Quality Assurance Cell One Day Hands-on Workshop on “Software for Chemistry and Materials by Nyro Research India.

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RESOURCE PERSON

Mr. Sreejit Soman, Application Scientist, Nyro Research India.



WORKSHOP AGENDA

Training session is tailored to meet expectations for computational chemistry, physics, nano science, polymer science, materials science including metallurgy and fluid thermodynamics

THEORY I - 45 MIN COMPUTATIONAL CHEMISTRY

Predicting structure, reactivity (catalysis), and spectral properties. NEGF, EDA, ZORA, QM/MM, GFN-1xTB, GBSA. DFTB module can treat molecular as well as periodic systems

DEMO I - 45 MIN ADF, DFTB CASE STUDIES

Transition State Searches for Click Reactions including geometry optimisation, DFT, EDA, TDDFT, IQA, NEGF, GW, Semi-empirical - MOPAC

THEORY II - 45 MIN MATERIALS SCIENCE

LCAO & Plane waves - Predict reactions, mechanical, optical and electronic properties. Advanced Molecular Dynamics and Monte Carlo simulations. (Re)parametrization tools and MD

DEMO II - 45 MIN BAND, REAXFF, FF TRAINING

Optical, mechanical, electronic properties, DoS, PEDA-NOCV, Electronic transport, TD-CDFT, ParAMS, Combustion Simulation, MD, QM/MM, Thermal & Ionic conductivity...

CASE STUDY - 30M VASP GUI, QE & COSMO-RS

Bumblebee for OLEDs, COSMO-RS pKa, polymer properties, ionic liquids, Python scripting using PLAMS, Phonon Band Structure, Kinetic Monte Carlo,

Our Softwares



For Hands-on Workshops:

- Windows/Mac OSX/Linux
- Laptop/Desktops 64bit
- 4GB RAM, Core i3/Ryzen 3 series CPUs with 5GB HDD storage required for software installation.
- Tutorials and example files will be shared.
- Training license with software links will be shared to registered attendees.

About VIT- Quality Week

Ensuring quality in higher educational institution is a bottom-up approach wherein every stake holder should be conscious of their role in contributing towards quality in the teaching-learning process, research, innovation, extension and governance. Organisational excellence is achieved only through quality individuals who can always be relied upon to do every activity in a right manner and consistently dedicate their full potential. With this in mind, VIT-IQAC in collaboration with all the academic and administrative units of VIT, strives to promote and ensure quality culture among all the stakeholders of the institute by organizing the fourth edition of VIT Quality Week' from 2nd to 6th March, 2026. The main objective of the Quality Week celebration is to raise awareness on quality assurance, sustenance, enhancement and enrichment initiatives among the stakeholders and to encourage them to adopt high-quality standards in education and research. It is also an opportunity for the institution to reflect on its quality practices and commit to a continuous quest for excellence, which will use in credibility to individuals and VIT. The theme for the Quality Week is "QUALITY: Drive for Innovations and Sustainability". Several events and activities focusing on learning and showcasing quality concepts have been planned during the quality week to ensure that the stakeholders of the HEI become quality conscious and be responsible for fostering a quality culture in the institute.

Venue



V. O. C Gallery II, 2nd floor, TT-building, VIT, Vellore, Tamil Nadu.

Register at

Date 6th March, 2026
09:30 AM - 05:30 PM

Register for

INR 150 Only + GST
(Non-refundable)

Register by

5th March, 2026

<https://events.vit.ac.in/>