



Five Days Hands-On Training on Density Functional Theory & its Applications using Gaussian 16

Organized by

Centre for Functional Materials,
Vellore Institute of Technology
and SCUBE Scientific

7 to 11th Nov 2022



Gaussian 16

Organizing Committee

Chief Patron:

Dr. G. Viswanathan

Chancellor

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Convener:

Dr. R. Ezhil Vizhi, Director, CFM

Coordinator:

Dr. Palanisami N. Professor, CFM

For more information:

Coordinator: **Dr. Palanisami N.**

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Access: <https://vit.ac.in/center/all-events/cfm>

Address:

Centre for Functional Materials,
Vellore Institute of Technology,
Vellore, 632014, India.

Lecture and Hands-on Sessions

Lecture :

Potential Energy Surface (PES)

Geometry Optimizations

Gaussian job files

Vibrational Spectroscopy

Thermochemistry

Methods in Gaussian (DFT, MM,
Semi-Empirical)

Solvation Methods

Model Chemistry

Gaussian Output

Hands-on Session :

Building Molecules

Running Electronic Structure Calculations

Visualizing Spectra & Surfaces

Investigating Chemical Reactions & Visualizing
Orbitals

Interested participants should register using the following Link :

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

Registration Fees : Rs. 2500 /- (Including GST)

Note:

- Registration deadline: 4th Nov-2022
- Participant confirmation on first come first serve basis
- Accommodation will be provided for external participants based on their request with additional charges
- E-book on Gaussian 16, Participation Certificate, Program kit, and Snacks will be provided
- Participants are requested to bring their laptop with charger

About VIT

VIT was founded in 1984 as Vellore Engineering College by the Hon. Chancellor Dr. G. Viswanathan with the aim of providing quality higher education on par with international standards. It persistently seeks and adopts innovative methods to improve the quality of higher education on a consistent basis. National Assessment and Accreditation Council (NAAC) has re-accredited (IV cycle) with a CGPA of 3.66 on a seven-point scale at 'A⁺⁺' Grade. VIT has been ranked 10th in Research, 12th in Engineering Category, 9th in University Category and 18th in the Overall Category by the MHRD-NIRF Ranking 2022.

About CFM

The Centre for Functional Materials (CFM) at VIT, Vellore was established in Dec. 2016 as a Centre for Crystal Growth. It was renamed and reorganized in NOV. 2020. The centre intends to prioritize the research of national interest by highlighting new findings and discussing current trends in specific domains. Here, we explore different classes of functional materials ranging from semiconductors to polymers and molecular crystals to nanoparticles.

About SCUBE

It is a renowned distributor of leading-edge scientific software in the field of Computational Chemistry, Biology, Mathematical Modeling, Statistical Analysis, Data Mining and Market Research, collaborating with a wide range of companies across the globe such as Gaussian Inc, Wolfram Research Inc and PerkinElmer Informatics to name a few. SCUBE Scientific Software Solutions Pvt Ltd is proud to announce that it has been awarded the Quality in Business Certification from the International Trade Council.

About Workshop

Density Functional Theory (DFT) has been used worldwide for geometry optimization, energy minimization, spectroscopic parameters, property calculations, etc. in all branches of science. This training programme will provide the fundamental knowledge about DFT to the participants to utilize Gaussian 16 software. The program will also be very beneficial and important for Research Scholar and Masters Students who are working in the area of DFT theory. The experienced trainers from SCUBE 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 the ample chance to learn new approaches in DFT.

Speakers and Trainers



Mr. Charitra Gour received his Masters in Pharmacy (Pharmaceutical Chemistry) from Amity University, Noida. Bachelor in Pharmacy from MJP Rohilkhand University Campus, Bareilly. He has delivered various talk training on various scientific software in CSIO Chandigarh, Guwahati University, IIS Jaipur, Central University of Jammu, Delhi University, Pune University, IIT Patna, Manipal University, NIT Manipur, MNIT Jaipur, BPCL India, TheraChem research, IIT Bhilai, University of Mysore, Mangalore University, ICT Hyderabad, Indian Institute of Petroleum Dehradun and various other educational institutes so far.



Mr. Bobby Solanki received his Masters and Bachelor from Chemistry, Sharda University, Greater Noida, U.P, India. He has delivered the training on various scientific software in CSIR-CDRI Lucknow, NIPER Raebareli, IIT Bombay, IIT Kanpur, IISER, Berhampur, National Chemical Laboratory (NCL) Pune, Shiv Nadar University Greater Noida, Sharda University Greater Noida, Delhi University, and various other educational institutes so far.