insilicology

3 Days Hands on Crash Course on

DFT ANALYSIS

Sign Up Now!

insilicology.org

wp @ +880 1987718298

insilicology@gmail.com

Follow insilicology

When & Where

COURSE DURATION (3 DAYS)
Dates : 12/15/20th July

TIME: 11.00 P.M.
GMT- 6.00

MODE: ONLINE
Zoom/ Google Meet

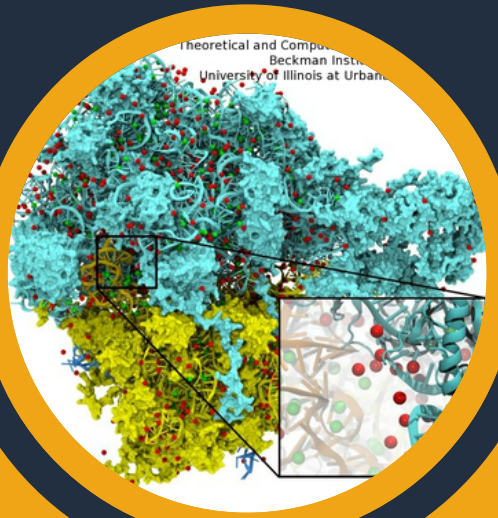
LANGUAGE
English

COURSE FEE
USD $50

"Meeting link will be share after registration"

Enroll Now!

For Registration
Scan or Click



"ONE COURSE ALL YOU NEED TO MASTER DFT ANALYSIS"

Welcomen

This Hands-On DFT Analysis Course is designed for students, researchers, and professionals seeking a practical foundation in quantum chemistry and reactivity analysis. Whether you're aiming to publish impactful research, advance in academia, or innovate in pharmaceuticals or materials science, this course provides essential skills in DFT and molecular modeling.

Far beyond a typical online course, it offers a guided, hands-on learning experience using real datasets and industry-standard tools like Gaussian, GaussView, Gabedit, and Avogadro

Course modules:

01 Introduction to DFT

02 Software & Molecular Setup

03 Basis Sets & Functionals

04 Geometry Optimization

05 Frequency & Thermochemical Calculations

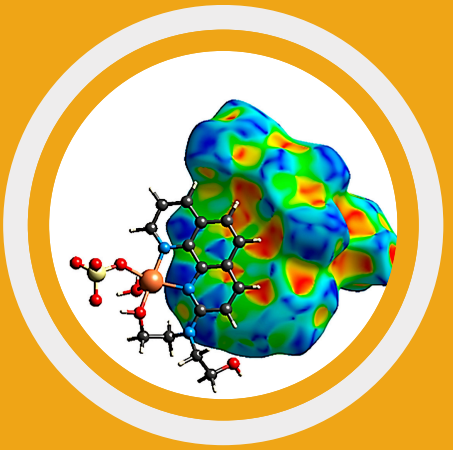
06 IR & Raman Spectra Simulation

07 HOMO–LUMO & Orbital Analysis

08 Reactivity Descriptors

09 Post-Processing Tools

10 Speed Up Your DFT Calculations



Why Choose This Course

- Structured for absolute beginners and intermediate learners
- Live, guided walkthroughs — not just pre-recorded videos
- Learn industry-relevant tools: Gaussian, ORCA, Avogadro, etc.
- Affordable and high-value compared to expensive university workshops or private trainings
- Lifetime access and support
- Certification upon completion
- Designed with a publication-focused approach

Enroll Now!

Course Modules

Module 1: Fundamentals of DFT and Quantum Chemistry

- Introduction to DFT concepts
- Key terms and approximations
- Applications in modern computational chemistry

Module 2: Software and Molecular Setup

- Installation and interface overview
- Building and optimizing molecular structures
- File formats and input preparation

Module 3: Basis Sets and Functionals

- Types of basis sets (STO-3G, 6-31G, etc.)
- Understanding exchange–correlation functionals
- Choosing appropriate combinations for accuracy

Module 4: Geometry Optimization

- Optimizing molecules using Gaussian/ORCA
- Convergence criteria and output interpretation
- Troubleshooting failed optimizations

Module 5: Frequency and Thermochemical Calculations

- Vibrational analysis and zero-point energy
- Thermodynamic corrections
- Identifying minima and transition states

Module 6: Molecular Orbital and Electronic Structure Analysis

- HOMO-LUMO, bandgap, and frontier orbital theory
- Orbital visualization using Multiwfn and ChemCraft
- Electrostatic potential maps

About the Instructor

The course is conducted by **Tawsif Al Arian**, a researcher affiliated with the Department of Pharmacy, Faculty of Biological Science Jahangirnagar University. With deep academic training and practical expertise in quantum chemistry and DFT-based simulations, Arian has mentored students and collaborators in computational molecular research.

He is the founder of Insilicology, an initiative offering advanced online training in computational chemistry and molecular modeling.

Course Modules

Module 7: Reactivity Descriptors and Conceptual DFT

- Global and local reactivity descriptors
- Fukui functions and dual descriptors
- Chemical hardness, potential, and electrophilicity

Module 8: Solvent Effects and Population Analysis

- Using PCM/SCRF models for solvation
- NBO and Mulliken charge analysis
- Dipole moments and polarizability

Module 9: Data Presentation and Publication Readiness

- Extracting publication-quality graphs and tables
- Formatting computational results

Module 10: Transition State Search

- Basic principles of TS search
- Tools and techniques for TS identification
- Verifying imaginary frequencies
- Creating figures for thesis, papers, and presentations
- Tips for publishing DFT results

Software Used:

- **gaussian**
- **gabedit**
- **gaussview**
- **avogadro**

Enroll Now!

About the Instructor

NAME: Tawsif Al Arian
BACKGROUND: B.Pharm (Professional)
Dept: Department of Pharmacy
Uni: Jahangirnagar University

CONTRIBUTION:

- iGEM Bangladesh Team 2024 (Bioinformatics Team Lead)
- iGEM Bangladesh Team 2025 (Advisory Board)
- IFCR Bangladesh (RA)

Research Interest: Anti-HIV agents targeting CCR5 and CXCR4 co-receptors, targets in idiopathic pulmonary, Ionic-liquid simulation, ML model and LAAMPS based projects

Course Details

- Duration: 3 Days
- Dates: 12th / 15th / 20th July 2025
- Time: 11:00 PM (GMT+6)
- Platform: Zoom / Google Meet
- Language: English
- Certificate: Provided (Digital PDF)
- Seats Available: Only 15 per batch
- Mode: Live + Recorded Access

COURSE FEE
USD $50

Group Offer: $40 USD per person for 3 or more registrations from the same institution (20% Discount)

Registration Process:

Fill out the form:

https://insilicology.org/enroll/dft

Or scan the QR code:

Or message us directly:

insilicology.org

wp @ +880 1987718298

insilicology@gmail.com

Follow insilicology

About Insilicology

Insilicology is an independent education and research-driven initiative dedicated to making computational chemistry and bioinformatics accessible and impactful. Our mission is to empower students, researchers, and institutions through hands-on, software-oriented training and support in modern in silico techniques.

We specialize in Density Functional Theory (DFT), quantum simulations, and reactivity analysis, along with a wide suite of services including:

- Molecular Docking & Molecular Dynamics Simulations
- QSAR Modeling & ADMET Prediction
- Network Pharmacology & Vaccine Design
- Bioinformatics & Computer-Aided Drug Design (CADD) &
- Others