SHARDA UNIVERSITY
Beyond Boundaries

NAAC A+ ACCREDITED

SHARDA SCHOOL OF ENGINEERING & SCIENCE

(Sharda University Local Chapter for Indian Society of Chemists and Biologists)

Department of Chemistry & Biochemistry

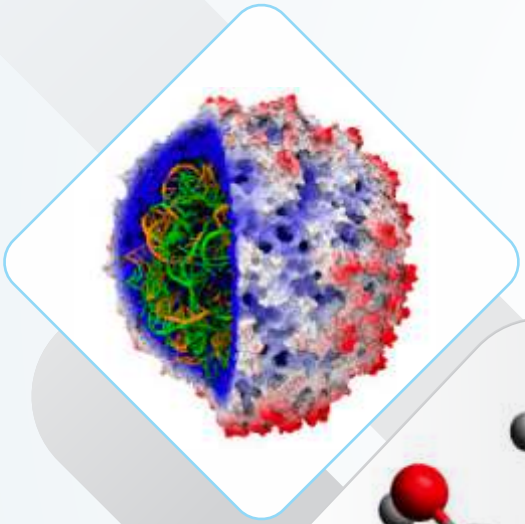
Organizes

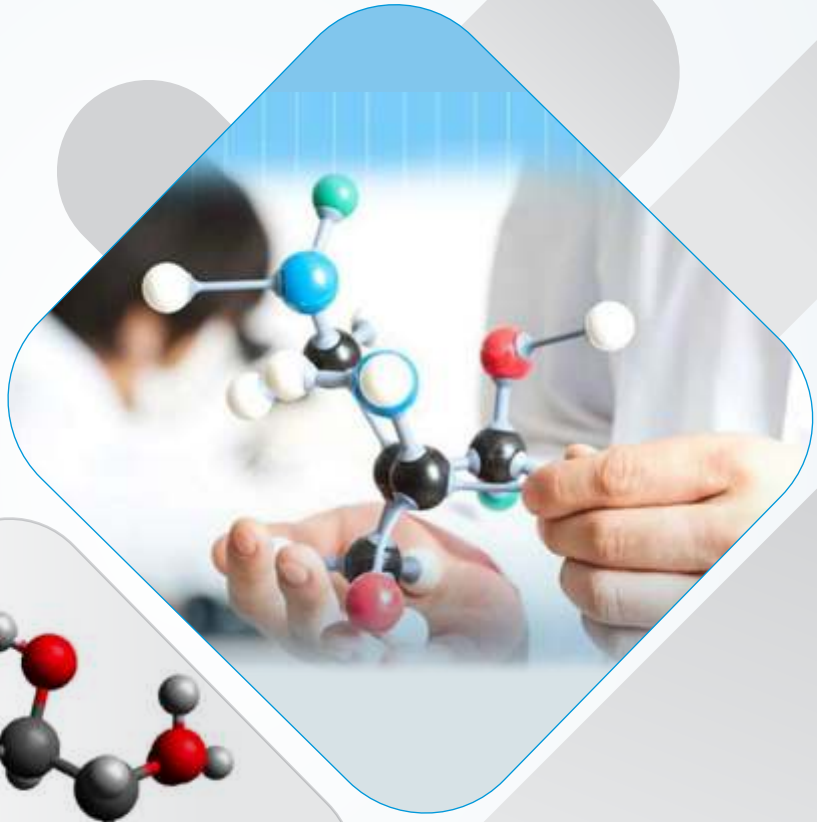
Five Days Workshop on

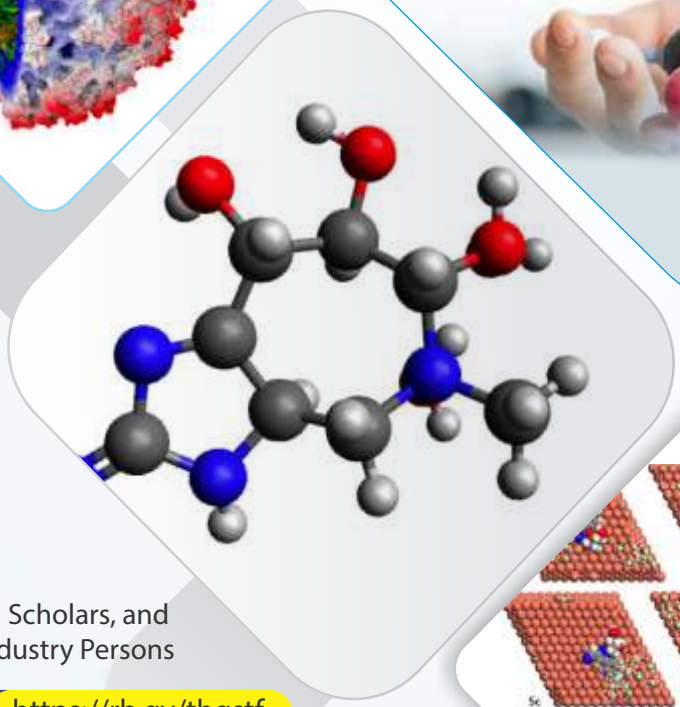
MOLECULAR MODELLING AND DFT COMPUTATION USING ORCA

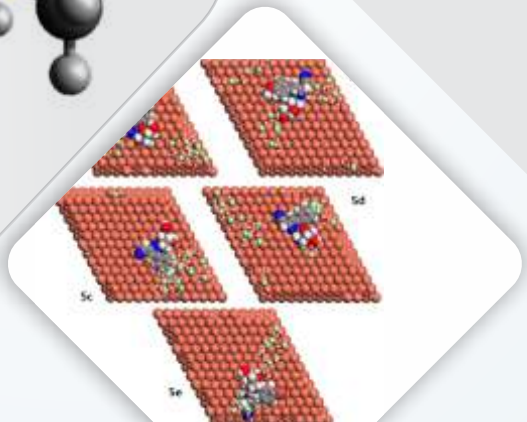
17th to 22nd April, 2025

3:00 PM to 6:00 PM









Eligibility: Research Scholars, and Faculty Members/Industry Persons

Registration link https://rb.gy/thqstf

ABOUT THE WORKSHOP

Department of Chemistry & Biochemistry, SSES, Sharda University, Greater Noida organizes a five days "Workshop on Molecular Modelling and DFT Computation using ORCA" on April 17-22, 2025. This workshop addresses the growing need of computational chemistry into academic research frameworks. From hands-on training to data analysis, this workshop will equip participants with cutting-edge tools and methodologies, fostering a culture of computation-driven innovation in academia.

KEY THEME

- Impact of Computational Chemistry and Density Functional Theory on chemical education.
- Strategies for promoting Research-Based Learning (RBL) and Outcome-Based Education (OBE).
- Faculty Development Programs (FDP) which empowers faculty members with the knowledge and skill necessary to develop their research.
- Institutional development for holistic education.

KEY OBJECTIVES

- To develop awareness of the theoretical and computational chemistry
- To be familiar with the applications of computational chemistry
- To get hands-on training on molecular modeling
- To be able to perform DFT computation using ORCA

HIGHLIGHTS

DAY-1 (17 April 2025)

- Introductory session about Indian Society for Chemists and Biologists (ISCB) by Prof. P. M. S. Chauhan, General Secretary of ISCB
- Brief introduction about density functional theory (DFT), functional, basis sets, and input file.
- Computational set up of ORCA and gOpenMol software packages.
- Use of open source software ChemDraw 3D and Mercury in computational modeling.
- 3D modeling of molecules and preparation of corresponding coordinate files.

DAY-2 (18 April 2025)

- Handling of X-ray single crystal files.
- Modifying the geometry of the molecules using reference crystal file.
- Preparation of input files using different key factors
- Geometry optimization computation and extraction of data from output file.
- Visualize the energy-optimize geometry of a molecule.

DAY-3 (19 April 2025)

- Basis set used for transition metals
- Preparation of input files for some complex molecules.
- Extraction of chemical data from output file.
- Visualization and further calculations

DAY-4 (21 April 2025)

- Time-dependent density functional theory (TDDFT) computation using coordinates of energy optimized geometry.
- Extraction of molecular orbitals and their energy from the output file.
- Extraction and visualization of isodensity plot for molecular orbitals
- Comparison of molecular orbital's energy, HOMO-LUMO gap calculation etc.

DAY-5 (22 April 2025)

- Extraction of electronic absorption spectral data from TDDFT output file.
- Plotting of calculated electronic absorption spectrum
- Calculation and interpretation of band energy
- Practice and doubts clearing sessions

PREREQUISITES

Personal laptop (MS Windows), Open source software (ChemDraw 3D, Mercury, Origin)

REGISTRATION FEE:

Participants	Sharda University	Other than Sharda University
Research Scholar	Rs. 500/- (including GST)	Rs. 750/- (including GST)
Faculty members / Industry persons	Rs. 1000/- (including GST)	Rs. 1250/- (including GST)

IMPORTANT DATES

Last Date for Registration: **16 April, 2025** Start of the Workshop: **17 April, 2025** End of the Workshop: **22nd April, 2025**

Registration Link: https://rb.gy/thqstf

Mode: Online

QR Code for Payment

Certification: *After completion the participants will be eligible for the certificate.*

CHIEF PATRONS

Shri. P. K. Gupta
Hon. Chancellor, Sharda University

Shri. Y. K. Gupta
Hon. Pro- Chancellor, Sharda University

PATRONS

Prof. (Dr.) Sibaram Khara
Vice - Chancellor, Sharda University

Prof. (Dr.) Parma Nand
Pro-Vice Chancellor, Sharda University

CO-PATRON

Prof. Bhuvnesh Kumar
Dean Research,
Sharda University

CONVENOR

Dr. Anupam Agarwal
Ph.D, HOD & Associate Professor,
Department of Chemistry & Biochemistry,
SSES, Sharda University,
Greater Noida, U.P.

Dr. P. M. S. Chauhan
Ph.D, FRSC
Ex-Chief Scientist and Professor (AcSIR)
Medicinal and Process Chemistry Division,CDRI, Lucknow 226031
General Secretary, Indian Society of Chemists and Biologists (ISCB)

ORGANIZING SECRETARY AND TRAINER

Dr. Suman Mallick
Ph.D, Assistant Professor,
Department of Chemistry & Biochemistry,
SSES, Sharda University

COORDINATOR

Dr. Priya Das
Ph.D, Assistant Professor,
Department of Chemistry & Biochemistry,
SSES, Sharda University