

Understanding Chemistry using Software

Molecular Modeling software provides an excellent and innovative option to understand the basics of Chemistry including macromolecules and biomolecules. With the help of such software, one can visualize the molecules, have an understanding of electronic distribution, study various properties of molecules like measurements, bond order, dipole moment etc. and visualize HOMO (Highest Occupied Molecular Orbital), LUMO (Lowest Unoccupied Molecular Orbital) and ESP (Electrostatic Potential) maps.

Learning Objectives:

The students will learn to use online Molecular Modeling software MolView, JMol, Avogadro and ArgusLab involving basic structure drawing and calculation of energy and properties like geometrical properties, bond order, charges, and HOMO, LUMO and ESP plots.

Learning Outcomes:

This course would help students to better understand the basics of Chemistry and would be an added advantage for them since molecular modelling is widely used by scientists around the world to solve scientific problems including drug designing for prevalent diseases.

Module 1: Hands-on session on MolView (6 Hours)

2D and 3D molecule builder with different representations, gives details of the molecule along with spectra available

Module 2: Hands-on session on JMol (7 Hours)

3D molecular structure building involving animations, vibrations, surfaces, orbitals, schematic shapes for secondary structures in biomolecules, measurements of bond lengths, angles and dihedral angles

Module 3: Hands-on session on Avogadro (7 hours)

A molecule editor and visualizer used for molecular modeling, bioinformatics, materials science, and related areas.

Module 4: Hands-on session on ArgusLab (10 Hours)

Molecule modeling, graphics and drug design software involving basic geometry optimization and energy calculations, surfaces, ESP plots, visualization of HOMO and LUMO, structural measurements