

Computational Methods (Theoretical Approaches)

Density Functional Theory (DFT)

Used to calculate electronic structure, energies, and reactivity of molecules and materials.

Molecular Dynamics (MD)

Used to study time-dependent behavior, stability, and motion of atoms and molecules.

Monte Carlo Method

Used to predict thermodynamic and equilibrium properties via random sampling.

Independent Gradient Model (IGM)

Used to visualize and analyze non-covalent interactions in molecular systems.

Hartree-Fock Method (HF)

Used to approximate electronic structure using wavefunctions (baseline quantum method).

Ab Initio Method

Used to predict molecular properties from first principles without empirical data.

Quantum Mechanics/Molecular Mechanics (QM/MM)

Used to model large systems by combining accurate quantum regions with efficient classical regions.

Finite Element Method (FEM)

Used to solve complex engineering and physical problems (e.g., stress, heat transfer).

Computational Fluid Dynamics (CFD)

Used to simulate fluid flow, mass transfer, and heat transfer in systems.

Software (Simulation & Modelling Tools)

Materials Studio

Used for molecular and materials modeling, including DFT, MD, and Monte Carlo simulations.

COMSOL Multiphysics

Used for multiphysics simulations (heat transfer, fluid flow, electromagnetics) using FEM.

ANSYS 2026

Used for engineering analysis such as structural mechanics, CFD, and thermal simulations.

Gaussian

Used for quantum chemical calculations (DFT, HF) to study molecular structure and reactions.

VASP

Used for DFT-based simulations of solid-state materials and surfaces.

LAMMPS

Used for large-scale MD simulations of materials and complex molecular systems.

GROMACS

Used for fast MD simulations, especially for biomolecules like proteins and lipids.

Fluent

Used for simulating fluid flow, heat transfer, and mass transport processes.

VESTA

Used for 3D visualization and analysis of crystal structures, electron density maps, and volumetric data (e.g., from DFT calculations); widely applied in materials science and solid-state chemistry.