# Introduction to Computational Chemistry

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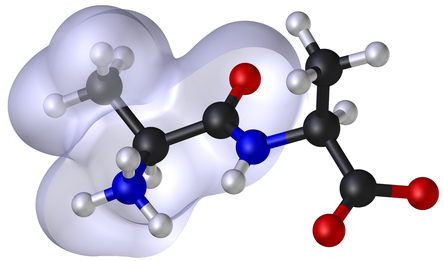
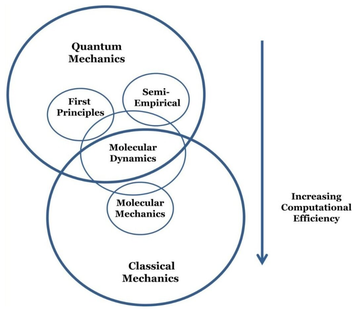
## What's Computational Chemistry ?



It combines principles from chemistry, physics, mathematics, and computer science to investigate the properties and behavior of molecules, reactions, and materials. The primary goal of computational chemistry is to provide insights into chemical phenomena that are difficult or impossible to observe experimentally.

## Methods

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### Molecular Mechanics

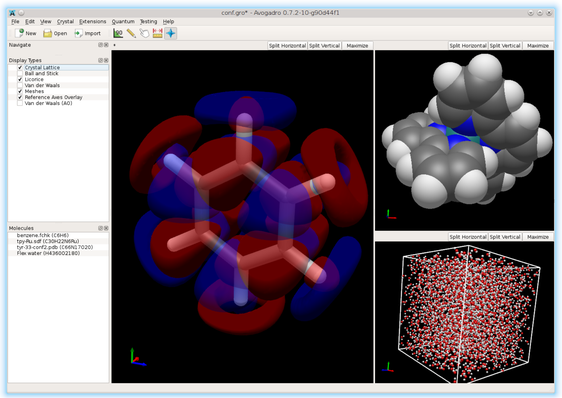
Molecular Mechanics is a computational approach that simplifies the modeling of molecular structures by approximating the interactions between atoms using classical mechanics principles.

### Quantum Mechanics

Quantum Mechanics is a more advanced computational method that considers the wave-like nature of electrons. In Quantum Chemistry, the Schrödinger equation is solved to determine the electronic structure of molecules.

## Tools and Softwares

1. Visualisation Tool
   1. VIAMD
   2. Avogadro
   3. JMol
2. Calculations Tools
   1. ORCA
   2. Gaussian
   3. NWChem



```
   23. D(H    6,C    1,C    8,H    3)   -180.00  0.000000   -0.00   -180.00
   24. D(H    6,C    1,C    8,H    4)     60.00  0.000000   -0.00     60.00
   25. D(H    7,C    1,C    8,H    2)   -180.00  0.000000   -0.00   -180.00
   26. D(H    7,C    1,C    8,H    3)     60.00 -0.000001    0.00    -60.00
   27. D(H    7,C    1,C    8,H    4)    -60.00 -0.000001    0.00    -60.00
   28. D(H    5,C    1,C    8,H    2)     60.00  0.000001   -0.00     60.00
   ----------------------------------------------------------------------------

         ************************************************************
         *                                                          *
         *          GEOMETRY OPTIMIZATION CYCLE   3                 *
         *                                                          *
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CARTESIAN COORDINATES (ANGSTROEM)
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  C      -0.685485    1.712874    0.000003
  C       0.654262    2.468801   -0.000003
  H      -0.586380    0.705695   -0.455890
  H      -1.457135    2.265507   -0.575496
  H      -1.072250    1.576056    1.031379
  H       1.041024    2.597615   -1.031381
  H       1.425908    1.908164    0.575496
  H       0.555157    3.467979    0.455891

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CARTESIAN COORDINATES (A.U.)
---------------------------------
  NO LB      ZA    FRAG     MASS         X          Y          Z
   0 C     6.0000    0    12.011   -1.295379    3.236862    0.000006
   1 C     6.0000    0    12.011    1.236375    4.650240   -0.000006
   2 H     1.0000    0     1.008   -1.108099    1.333570   -0.861506
   3 H     1.0000    0     1.008   -2.753586    4.281187   -1.087530
   4 H     1.0000    0     1.008   -2.026259    2.978314    1.949025
```

## Theoretical Explanations

1. Schrödinger's Time-Independent Equation :

$$\hat{H}\Psi = E\Psi$$

   Describes the quantum state of a system, where $\hat{H}$ is the Hamiltonian operator, $\Psi$ is the wave function, and $E$ is the energy. Solving this equation provides information about electronic structure and properties.
2. Hartree-Fock Equations :

$$\hat{H}_{\text{HF}}\Phi_i = \varepsilon_i\Phi_i$$

   Solves for the electronic wave functions ($\Phi_i$) and energies ($\varepsilon_i$) in a self-consistent field.
3. Density Functional Theory (DFT) :

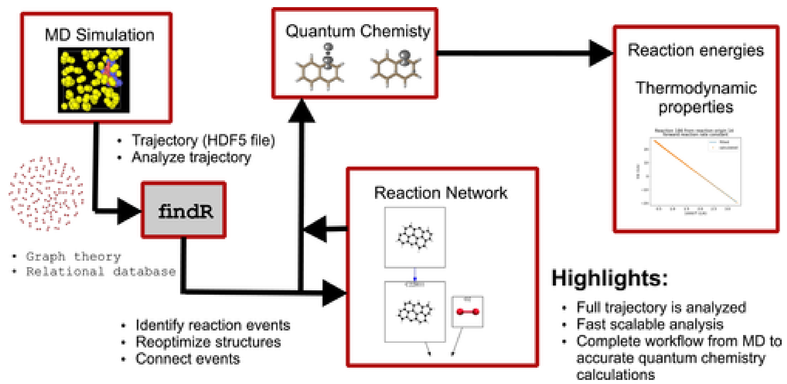
$$E_{\text{DFT}} = T_s[n] + E_{\text{ee}}[n] + E_{\text{ext}}[n] + E_{\text{XC}}[n]$$

   Describes the total energy in terms of the kinetic energy, electron-electron interaction, external potential, and exchange-correlation energy. DFT is widely used for electronic structure calculations.
4. Molecular Mechanics Force Field Equation :

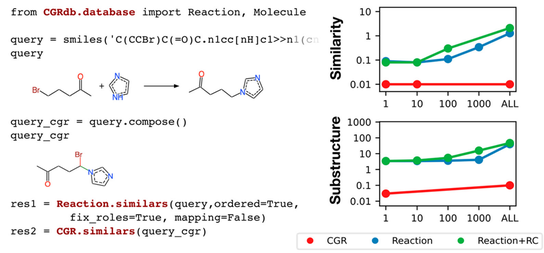
$$E_{\text{MM}} = \sum_{\text{bonds}} K_r(r - r_0)^2 + \sum_{\text{angles}} K_\theta(\theta - \theta_0)^2 + \sum_{\text{dihedrals}} K_\phi(1 + \cos(n\phi - \phi_0))$$

   Describes potential energy in terms of bonded and non-bonded interactions, allowing molecular dynamics simulation.

## Project Workflow



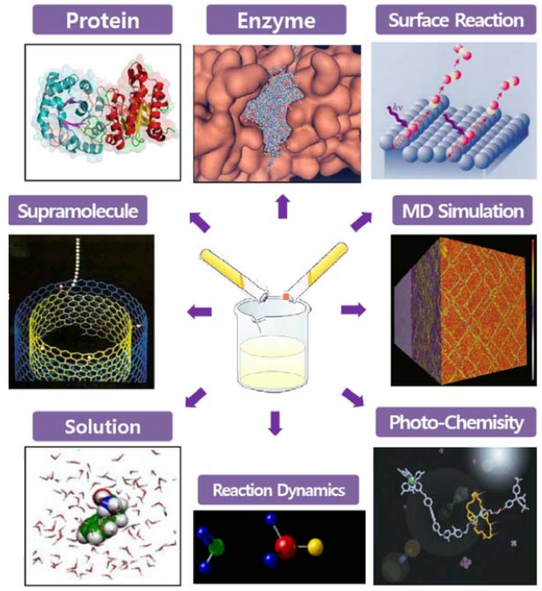

## Python and ML




Libraries :

1. Numerical Computing - NumPy and SciPy
2. Quantum Chemistry - PySCF , Psi4
3. Machine Learning - scikit-learn, RDKit

## Applications




This field is instrumental in drug discovery, simulating molecular interactions pharmaceutical development. It shapes nanotechnology and energy storage by designing materials . Catalysis benefits from elucidated reaction mechanisms. Environmental science leverages computational models to predict pollutant behavior and design eco-friendly materials.

## Future Prospects

1. Integration of Machine Learning
2. High-Performance Computing
3. Advancements in Quantum Computing
4. Interdisciplinary Collaborations
5. Continued Software Development