Computational Chemistry: Foundation and Tools

Proposed Credits: 1-1-0
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Term: January 2026

Prerequisite: Basic Quantum chemistry

Course Aim

To give an idea of basic computational chemistry and familiarize with ORCA software.

Topics to be Covered

1. Foundations of Electronic Structure Theory

- Many-electron problem and approximations
- Hartree-Fock method and Basis sets

2. Density Functional Theory

- Kohn-Sham theorems
- Exchange-correlation approximations (LDA, GGA, hybrids)
- Strengths and limitations

3. Practical Computation Using ORCA and Avogadro

- Installing and navigating packages
- Input structure, keywords, job types
- Geometry optimization and frequencies
- Computing molecular properties and different spectra. Relating them to molecular structure
- Homo Lumo Visualization
- Adding implicit solvation model to understand the effect of solvent
- Searching the transition state for a given set of reactant and product.

4. Survey of Advanced Computational Techniques
A fast overview of broader landscape:

- Molecular dynamics: classical and ab-initio

References

- Jensen, *Introduction to Computational Chemistry*
- Levine, *Quantum Chemistry*
- ORCA and GAUSSIAN user manuals