CH-326 Computational Chemistry

Credit Hours: 2-1

Pre-requisite: Nil

Course Objectives

1. This course introduces undergraduate students to the fundamental concepts, tools, and techniques of computational chemistry. The focus is on applying computational methods to visualize, simulate, and analyze molecular structures and chemical processes with minimal mathematical complexity. Students will gain hands-on experience with software tools to explore real-world applications in drug design, materials science, and environmental chemistry.

Course Contents

2. Introduction to Computational Chemistry: Importance and scope in modern chemistry, Role in research, industry, and academia, Overview of theoretical foundations (quantum vs. classical models), 2. Molecular Mechanics and Force Fields, Atoms as balls and springs, Energy minimization and molecular geometry, Basic force fields: UFF, MMFF94, AMBER, 3. Visualization and Molecular Modeling Tools: Introduction to software: Avogadro, ChemDraw, GaussView, Drawing and optimizing molecular structures, Measuring bond lengths, angles, and torsions, 4. Basics of Quantum Chemistry Methods: Molecular orbitals, HOMO-LUMO concept, Semi-empirical and ab initio methods (overview only), 5. Simulating Chemical Reactions and Properties: Geometry optimization and vibrational frequency analysis, Dipole moment, charge distribution, and reactivity predictions, Real-life examples from pharmaceuticals and pollutants.

Course Outcomes

By the end of this course, the students will be able to:

3. Describe key computational methods used to model molecular structures and simulate chemical behavior.
4. Apply molecular modeling and visualization tools to study molecular geometries and reaction mechanisms.
5. Analyze chemical properties (e.g., energies, dipoles, charges) using basic quantum and classical techniques.
6. Evaluate the role of computational tools in fields such as drug design,

environmental chemistry, and materials science.

7. Conduct simple computational experiments and interpret the results in a chemical context..

Relevant Experiments

1. Molecular Drawing and Visualization: Create and visualize methane, ethanol, benzene, and amino acids.
2. Geometry Optimization Using Molecular Mechanics: Optimize water, acetic acid, and cyclohexane in chair and boat conformations.
3. Bond Length and Angle Analysis: Analyze bond parameters of ethene, butane, and glucose.
4. Molecular Orbital and HOMO-LUMO Analysis: Compare the HOMO-LUMO gap of ethene vs. ethyne, or carbonyl vs. amine.
5. Charge Distribution and Electrostatic Potential Mapping: Analyze formaldehyde, aniline, and nitrobenzene.
6. Vibrational Frequency Calculation: Run vibrational analysis for water, CO_2, and NH_3; identify symmetric/asymmetric stretching.
7. Solvent Effect on Molecular Properties: Compare acetone in gas phase and in water using PCM model.
8. Conformational Analysis of n-Butane and Cyclohexane: Plot energy vs. dihedral angle (butane), chair-boat interconversion (cyclohexane).
9. Case Study Project: Molecular Property Prediction: Students choose a molecule (e.g., caffeine, ibuprofen, paracetamol) and report structure, charges, dipole moment, HOMO-LUMO gap, and IR spectrum.

Recommended Books

1. Jensen, F. (2016). Introduction to Computational Chemistry (3rd ed.). John Wiley & Sons. ISBN: 9781118825990.
2. Prasad, R. Y., & Pranita. (2021). Computational Quantum Chemistry (2nd ed.). CRC Press. ISBN: 9780367679699.
3. Sholl, D. S., & Steckel, J. A. (2022). Density Functional Theory: A Practical Introduction (2nd ed.). Wiley. ISBN: 9781119581727.
4. Boyd, R. D. (Ed.). (2023). Comprehensive Computational Chemistry. Elsevier. ISBN: 9780128219786.
5. Blinder, S. M. (2023). A Primer on Quantum Chemistry. Wiley. ISBN:

9781119829638.

6. Leszczynski, J., & Shukla, M. K. (Eds.). (2022). Practical Aspects of Computational Chemistry V. Springer. ISBN: 9783030936106.
7. Ul-Haq, Z., & Wilson, A. K. (Eds.). (2022). Frontiers in Computational Chemistry (Vol. 6). Bentham Science Publishers. ISBN: 9789815051904.