CH-834 Computational Chemistry and Molecular Design

Credit Hours: 3-0

Prerequisite: Nil

Course Objectives

This course is designed to bridge theoretical principles with real-world molecular modeling applications. It equips students with practical skills in quantum chemical and molecular simulation tools to investigate molecular properties, reactivity, and reaction mechanisms. Emphasis is placed on computational strategies and software rather than mathematical formalism, ensuring the course remains engaging and practice-oriented.

Course contents

1. Introduction to Molecular Modeling and Simulations: Scope and relevance in chemistry and materials science, Differences between molecular mechanics, semi-empirical, and ab initio methods, Overview of commonly used computational packages (Gaussian, ORCA, VASP, Avogadro, ChemCraft), 2. Quantum Chemistry in Action: Basis sets, functionals, and levels of theory, Energy minimization and geometry optimization, HOMO-LUMO analysis, charge distribution, and molecular orbitals visualization, Vibrational frequency calculations (IR, Raman predictions), 3. Reaction Mechanisms and Transition States: Transition state search methods, Intrinsic Reaction Coordinate (IRC) analysis, Case studies: SN2, pericyclic, and catalytic reactions, 4. Hybrid QM/MM Approaches: Theory and implementation, Applications in enzyme catalysis and drug design, Fragmentation and embedding methods

5. Molecular Dynamics and Conformational Analysis: Introduction to force fields (AMBER, CHARMM, OPLS), Conformational sampling and Boltzmann weighting, Application: protein-ligand interaction prediction, 6. Project Module & Applications: Computational screening of catalysts or ligands, Predicting thermodynamic parameters of novel molecules, Data interpretation from output files and visualization tools, Short projects using real research problems (e.g., battery materials, pharmaceuticals, CO_2 capture).

Course Outcomes

Upon successful completion, students will be able to:

Utilize advanced quantum chemical tools to predict molecular structures, energies, and reactivities.

Interpret computational results using visualization and analysis software for real-world chemical problems.

Apply simulation-based approaches (MD, QM/MM) to explore reaction pathways and dynamic behavior of molecules.

Design and carry out independent computational experiments, suitable for thesis-level or publication-quality research.

Integrate computational data with experimental insights in multidisciplinary research contexts.

Recommended Books

Essentials of Computational Chemistry, C. J. Cramer

Molecular Modelling: Principles and Applications, Andrew R. Leach

Exploring Chemistry with Electronic Structure Methods, Foresman and Frisch

Practical Introduction to Molecular Dynamics, Leach and Frenkel

Software Tools: Gaussian, ORCA, VASP, Avogadro, ChemCraft, GaussView, Multiwfn.