



University of Management and Technology, Lahore
School of Science
Department of Chemistry
Certificate Course

Course Title:

Computational Chemistry

By Dr. Naveen Kosar

Introduction:

This course will introduce participants to the fundamental concepts of computational chemistry and their practical applications. Participants will learn the basics of molecular modeling and simulation, quantum chemistry, and molecular dynamics simulations. Through hands-on exercises and project-based learning, students will gain experience with computational tools and techniques used in chemistry research.

Objectives:

- To provide an introduction to the concepts and applications of computational chemistry.
- To teach how to use computational tools and techniques to solve chemical problems.
- To develop skills in molecular modeling and simulation.
- To provide with an understanding of the principles of quantum chemistry and molecular dynamics simulations.
- To apply computational chemistry to solve real-world problems in chemistry research.

Learning Outcomes:

Upon completion of this course, participants will be able to:

- Understand the basic principles and applications of computational chemistry.
- Analyze and evaluate chemical problems using computational tools and techniques.
- Develop molecular models and simulate chemical systems using computational software.
- Apply principles of quantum chemistry and molecular dynamics simulations to solve chemical problems.
- Interpret and communicate computational results to inform experimental design and data analysis in chemistry research.

Duration:

Four weeks, two days a week. Monday-Tuesday 5 pm to 7 pm

Eligibility/Registration Criteria:

Students completed 14 years of science education.



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Course Outline:

Week	Lecture #	TOPICS
1	1	Overview of computational chemistry and its applications in chemical research
	2	Basic principles of molecular modeling and simulation, Introduction to computational software
2	1	Energy minimization and conformational analysis
	2	Force fields and molecular mechanics, Monte Carlo and molecular dynamics, Density functional theory
3	1	Examples of using computational chemistry to solve real-world problems in chemistry research i. Drug Design ii. Material Design iii. Catalysis
	2	Integration of computational and experimental techniques in chemistry research, Visualization and analysis of molecular models
4	1	Implementation of different software i. Gaussian ii. GAMESS
	2	iii. ORCA iv. Quantum Espresso

Evaluation Criteria:

Participation/ Attendance: (20%)

Quizzes: (40%)

Assignments: (40%)

Study Materials:

- "Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics" by Errol G. Lewars.
- Video lectures and readings will be provided through an online platform.



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- Computational software will be made available to participants for the duration of the course.