SIR SYED COLLEGE, TALIPARAMBA

(Affiliated to Kannur University)

Re-accredited by NAAC with A Grade

Kannur, Kerala, India-PIN 670142

SYLLABUS FOR ADD –ON COURSE

NAME OF THE ADD ON COURSE: **Introduction to Computational Analysis**

Offered By: Department of Chemistry

Name of the Course Co-Ordinator: Ms. Fasila PM

Board of Studies Members:

Chairman: Dr Biju AR

Members

1. Ms. Fasila PM
2. Ms. Shahabau P
3. Ms. Sarayu Jayadevan
4. Ms. Rahana Ameen (Assistant Professor & HoD Payyannur College)

Name of the course: Introduction to Computational Analysis

Course Description: This course introduces students to various computational chemistry methods, including Molecular Mechanics, Quantum Mechanics (Ab-initio, Hartree-Fock, Semi-empirical, and Density Functional), and the fundamentals of constructing basis sets for molecules.

Vision

To empower students with a profound understanding of computational chemistry methods and basis sets, fostering their ability to contribute to groundbreaking scientific discoveries and innovation in the field of molecular science

Mission

Our mission is to provide a rigorous and comprehensive education in computational chemistry methods and basis sets, equipping students with the knowledge and skills necessary to excel in academic and research endeavors

Programme Specific Outcomes (CSOs):

CSO1: Apply Molecular Mechanics principles to analyze and predict the structural and energetic properties of molecules and molecular complexes.

CSO2: Perform Quantum Mechanics calculations using appropriate software packages to calculate molecular properties.

CSO3: Conduct Ab-initio calculations and understand the influence of electron correlation on molecular energy and geometry.

CSO4: Implement semi-empirical methods to estimate molecular properties efficiently and recognize their limitations.

CSO5: Apply Density Functional Theory to compute molecular properties and interpret the results in the context of chemical phenomena.

CSO6: Demonstrate the ability to choose the most suitable basis set for a given quantum chemistry problem.

CSO7: Construct basis sets accurately, considering the specific requirements of different molecules.

CSO8: Identify and troubleshoot issues related to basis set convergence and recommend strategies for improvement.

Suggested Methodology for Teaching, Learning and Evaluation

Evaluation

Evaluation	**Weightage %**
External (Based on Theory and Practical exam)	80
Internal (Based on Internal test, assignment and Viva)	20

Name of Add on Course- : Introduction to Computational Methods of Analysis

Duration of the course	Course Code	Hours per week	Credit and Modules	Exam Hours
20 hrs	**AOCHE01CMP**	**2**		**3**

The course is structured to provide an introduction to Gausian 09 Programme with a focus on selected methods for computing energies and studying molecular properties. The course also includes a hands-on training for beginning users on the Gaussian 09 and GaussView 5 software packages.

Course Outcomes:

1. Learn to draw chemical structures using different softwares

2. Analyse the structure-property relations of various molecular systems

3. Interpret the IR spectrum of different molecules

Detailed Syllabus with module and hours

Module:1 – Methods in Computational Chemistry

Introduction to methods in computational chemistry- Molecular Mechanics, Quantum Mechanics- Ab-initio methods, Hartree- Fock Method, Semi-empirical methods, Density Functional Method. (10 Hours)

Module:2- Basis sets

Introduction to Basis sets- Slater –Type and Gausian-Type Orbitals. Classification of Basis Sets. Contruct Basis sets for water, carbondioxide, methane. (8 Hours)

Module 3- **Practical Considerations**

Designing Computational Experiments , Basics of Running Gaussian Calculations, DFT Geometries and Frequencies **,** Compute Energies**,** Geometry Optimization Minima Vibrational Spectroscopy , Anatomy of a Gaussian Input File, Study the format of Gaussian Output Files. (12 Hours)

REFERENCES:

1. Quantum Mechanics by G Aruldhas
2. Exploring Chemistry with Electronic Structure Methods Book by James B. Foresman
3. Methods of Electronic-Structure Calculations: From Molecules to Solids by Michael Springborg"
4. Essentials of Computational Chemistry by Christopher J. Cramer