- Teaching through audio-visual aids.
- Students are encouraged to participate actively in the classroom through regular presentations on curriculum based topics.
- As the best way to learn something is to do it yourself, practicals are planned in such a way so as to reinforce the topics covered in theory.

Assessment Methods:

- Presentations by individual student/ small group of students
- Class tests at periodic intervals.
- Written assignment(s)
- Objective type chemical quizzes based on contents of the paper.
- End semester university theory and practical examination.

Keywords:

Separation techniques, Solvent extraction, Ion-exchange, Optical methods, Flame Atomic Absorption and Emission Spectrometry, indeterminate errors, statistical test of data; F, Q and t tests. TGA.

Course Code: CHEMISTRY –DSE-5
Course Title: Molecular Modelling and Drug Design
Total Credits: 06 (Credits: Theory-04, Practical-02)
(Total Lectures: Theory- 60, Practical-60)

Objectives:

Objective of this course is to make students learn the theoretical background of principles of computational techniques in molecular modelling, evaluation and applications of different methods for various molecular systems, energy minimization techniques, analysis of Mulliken Charge & ESP Plots and elementary idea of drug design.

Learning Outcomes:

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

- Understand theoretical background of computational techniques and selective application to various molecular systems.
- Learn Energy minimization methods through use of different force fields.
- Learn ESP Plots by suitable soft wares, electron rich and electron deficient sites,
- Compare computational and experimental results and explain deviations.
- Carry out Molecular dynamics (MD) and Monte Carlo (MC) simulations on several molecules and polymers.
- Learn QSAR properties and their role in molecular modelling, cheminformatics and drug discovery.
- Perform Optimization of geometry parameters of a molecule (such as shape, bond length and bond angle) through use of software like Chem Sketch and Argus Lab in interesting hands-on exercises.

Unit 1:

Introduction: Overview of Classical and Quantum Mechanical Methods (Ab initio, Semi-empirical, Molecular Mechanics, Molecular Dynamics and Monte Carlo) General considerations.

Coordinate systems: Cartesian and Internal Coordinates, Bond lengths, bond angles and torsion angles, Writing Z -matrix (ex: methane, ethane, ethene, ethyne, water, H_2O_2 .

(Lectures: 8)

Unit 2:

Potential Energy Surfaces: Intrinsic Reaction Coordinates, Stationary points, Equilibrium points – Local and Global minima, concept of transition state with examples: Ethane, propane, butane, cyclohexane. Meaning of rigid and relaxed PES.

Applications of computational chemistry to determine reaction mechanisms.

Energy Minimization and Transition State Search: Geometry optimization, Methods of energy minimization: Multivariate Grid Search, Steepest Descent Method, Newton-Raphson method and Hessian matrix.

(Lectures: 12)

Unit 3:

Molecular Mechanics: Force Fields, Non-bonded interactions (van der Waals and electrostatic), how to handle torsions of flexible molecules, van der Waals interactions using Lennard-Jones potential, hydrogen bonding interactions, electrostatic term, Parameterization. Applications of MM, disadvantages, Software, Different variants of MM: MM1, MM2, MM3, MM4, MM+, AMBER, BIO+, OPLS.GUI.

(Lectures: 10)

Unit 4:

Molecular Dynamics: Radial distribution functions for solids, liquids and gases, intermolecular Potentials (Hard sphere, finite square well and Lennard-Jones potential), concept of periodic box, ensembles (microcanonical, canonical, isothermal – isobaric), Ergodic hypothesis. Integration of Newton's equations (Leapfrog and Verlet Algorithms), Rescaling, Simulation of Pure water – Radial distribution curves and interpretation, TIP & TIP3P, Typical MD simulation

Brief introduction to Langevin and Brownian dynamics

Monte Carlo Method: Metropolis algorithm.

(Lectures: 10)

Unit 5:

Huckel MO with examples: ethane, propenyl, cyclopropenyl systems, Properties calculated – energy, charges, dipole moments, bond order, electronic energies, resonance energies, Oxidation and reduction (cationic and anionic species of above systems)

Extension to Extended Huckel theory and PPP methods

***Ab-initio* methods:** Writing the Hamiltonian of a system, Brief recap of H – atom solution, Units in quantum mechanical calculations, Born-Oppenheimer approximation (recap), Antisymmetry principle, Slater determinants, Coulomb and Exchange integrals,

Examples of He atom and hydrogen molecule, Hartree-Fock method

Basis sets, Basis functions, STOs and GTOs, diffuse and polarization functions. Minimal basis sets

Advantages of ab initio calculations, Koopman's theorem, Brief idea of Density Functional Theory

(Lectures: 12)

Unit 6:

Semi-empirical methods: Brief idea of CNDO, INDO, MINDO/3, MNDO, AM1, PM3 methods. Other file formats – PDB. Visualization of orbitals – HOMO, LUMO, ESP maps.

QSAR: Structure-activity relationships. Properties in QSAR (Partial atomic charges, polarizabilities, volume and surface area, log P, lipophilicity and Hammet equation and applications, hydration energies, refractivity). Biological activities (LD50, IC50, ED50.)

(Lectures: 8)

Practical:

(Credits: 2, Laboratory periods: 60)

1. Plotting a 3D graph depicting a saddle point in a spreadsheet software.
2. Determine the enthalpy of isomerization of cis and trans 2-butene.
3. Determine the heat of hydrogenation of ethylene.
4. Compare the optimized C-C bond lengths and Wiberg bond orders in ethane, ethene, ethyne and benzene using PM3. Is there any relationship between the bond lengths and bond orders? Visualize the highest occupied and lowest unoccupied molecular orbitals of ethane, ethene, ethyne, benzene and pyridine.
5. Perform a conformational analysis of butane.
6. Compare the basicities of the nitrogen atoms in ammonia, methylamine, dimethylamine and trimethylamine by comparison of their Mulliken charges and ESP maps.
7. Compare the gas phase basicities of the methylamines by comparing the enthalpies of the following reactions:

$BH^+ + NH_3 \rightarrow B + NH_4^+$

where B = CH_3NH_2, $(CH_3)_2NH$, $(CH_3)_3N$

8. Arrange 1-hexene, 2-methyl-2-pentene, (E)-3-methyl-2-pentene, (Z)-3-methyl-2-pentene, and 2,3-dimethyl-2-butene in order of increasing stability.

9. Compare the optimized bond angles H_2O, H_2S, H_2Se using PM3.

10. Compare the HAH bond angles for the second row hydrides (BeH_2, CH_4, NH_3, H_2O) and compare with the results from qualitative MO theory.

11. (a) Compare the shapes of the molecules: 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2-propanol. Note the dipole moment of each molecule. (b) Show how the shapes affect the trend in boiling points: (118 ºC, 100 ºC, 108 ºC, 82 ºC, respectively).

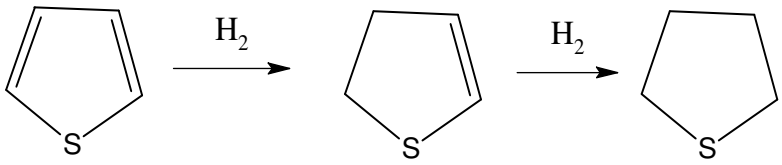
12. Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.

13. Plot the electrostatic potential mapped on electron density for benzene and use it to predict the type of stacking in the crystal structure of benzene dimer.

14. Predict the aromaticity of thiophene with respect to benzene by comparing the enthalpies of the following reactions:

    (a) Hydrogenation of benzene to 1,3-cyclohexadiene and then 1,3-cyclohexadiene to cyclohexene.

    (b)



15. Docking of Sulfonamide-type D-Glu inhibitor into MurD active site using Argus lab.

Note: Software: Argus Lab (www.planaria-software.com).

References:

Theory:

1. Lewars, E. (2003), **Computational Chemistry**, Kluwer academic Publisher.
2. Cramer, C.J.(2004),**Essentials of Computational Chemistry**, John Wiley & Sons.
3. Hinchcliffe, A. (1996),**Modelling Molecular Structures**, John Wiley & Sons.
4. Leach, A.R.(2001),**Molecular Modelling**, Prentice-Hall.

Practical:

1. Lewars, E. G. (2011),**Computational Chemistry**, Springer (India) Pvt. Ltd. Chapter 1 & 2.

2. Engel, T.; Reid, P.(2012),**Physical Chemistry**, Prentice-Hall. Chapter 26.

Teaching Learning Process:

Conventional methods of teaching i.e. lectures, PPTs, Hands on practice of molecule centric problems with maximum characterization parameters and recently designed lead drug molecules

Assessment Methods:

- Assignment based on Theoretical designing of small molecules of drug prospective
- Presentation on fundamentals of drug designing and molecular modelling
- Test
- Semester end examination

Keywords:

Molecular modelling, Quantum Mechanical Method, Cartesian Coordinates, Molecular Dynamics, Force Field, Software of Computational Chemistry.

Course Code: CHEMISTRY –DSE-6
Course Title: Polymer Chemistry
Total Credits: 06 (Credits: Theory-04, Practical-02)
(Total Lectures: Theory- 60, Practical-60)

Objectives:

The primary objective of this paper is to help the student to know about the synthesis, properties and applications of polymers.

Learning Outcomes:

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

- Know about history of polymeric materials and their classification
- Learn about different mechanisms of polymerization and polymerization techniques
- Evaluate kinetic chain length of polymers based on their mechanism
- Differentiate between polymers and copolymers
- Learn about different methods of finding out average molecular weight of polymers
- Differentiate between glass transition temperature (Tg) and crystalline melting point (Tm)
- Determine Tg and Tm
- Know about solid and solution properties of polymers
- Learn properties and applications of various useful polymers in our daily life.