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DISCIPLINE SPECIFIC ELECTIVE COURSE -12 (DSE-12): Computational Methods & Molecular Modelling

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Computational Methods & Molecular Modelling (DSE-12)	**04**	**03**	**--**	**01**	Class 12th with Physics, Chemistry and Mathematics	--

Learning Objectives

The Objectives of this course are as follows:

- To make students learn the theoretical background of computational techniques in molecular modelling.
- To give the different flavours of computational chemistry by the end of this course.
- To provide hands-on experience in molecular modelling on various software

Learning outcomes

By studying this course, the students will be able to:

- Explain the theoretical background of computational techniques and selective application to various molecular systems.
- Compare computational and experimental results and explain deviations.
- Perform Optimization of geometry parameters of a molecule (such as shape, bond length and bond angle) through the use of software like Chem Sketch and Argus Lab in interesting hands-on exercises.
- Perform analysis of molecular properties using various software.

SYLLABUS OF DSE-12

UNIT-1 : Introduction **(Hours: 6)**

Introduction to computational chemistry: Overview of Classical and Quantum Mechanical Methods (Ab initio, DFT, Semi-empirical, Molecular Mechanics, Molecular Dynamics, and Monte Carlo)

UNIT – 2: Potential Energy Surfaces **(Hours: 6)**

Intrinsic Reaction Coordinates, Stationary points, Equilibrium points – Local and Global minima, Geometry optimization and energy minimization, the concept of transition state with examples, Hessian matrix

UNIT – 3 : Molecular Mechanics & Molecular Dynamics **(Hours: 9)**

Molecular Mechanics

Force Fields (A brief explanation of all the terms of a basic force field), the basic idea of MM1, MM2, MM3, MM4, MM+, AMBER, BIO+, OPLS.

Molecular Dynamics

The concept of the periodic box, ensembles (microcanonical, canonical, isothermal – isobaric), steps in a typical MD simulation.

UNIT-4: Huckel Molecular Orbital Theory **(Hours: 6)**

Huckel MO with examples: ethene and propenyl systems, Properties calculated – energy, charges, bond order, electronic energies, resonance energies.

UNIT- 5: Computational Methods **(Hours: 18)**

Ab-initio methods

Antisymmetry principle, Slater determinants, SCF method, Hartree-Fock method.
Basis sets, Basis functions, STOs and GTOs, diffuse and polarization functions. Minimal basis sets, Basis set superposition error (BSSE) - Effective core potentials (ECP)
Advantages of ab initio calculations.

Density Functional Theory

A brief description of Density Functional Theory (DFT). Calculation of Electronic Properties in ground and Excited states

Semi-empirical methods

Basic idea about Zero differential overlap (ZDO) approximation

Some important concepts

Concepts of atomic charges, electrostatic potential maps, computation of thermodynamic properties and spectroscopic observables

Practical component

Practical: **Credits: 01**

(Laboratory periods:15 classes of 2 hours each)

1) Write the Z-Matrix of a given set of molecules.

2) Carry out geometry optimisation on H_2O, H_2S, H_2Se molecules compare the optimized bond angles and dipole moments from the results obtained. Obtain the ESP-mapped density surfaces and interpret the results obtained with reference to bonding in these molecules.

   Suggestive: A comparative analysis of results of the above exercise may be carried out using different quantum mechanical methods.

3) Calculate the energy of the following chemical species and arrange them in order of increasing stability.

   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.

4) Carry out geometry optimisation on the following chemical species and compare the shapes and dipole moments of the molecules.

   1-pentanol, 2-pentanol, 3-pentanol, 2-methylbutan-1-ol, 3-methylbutan-1-ol, 2-methylbutan-2-ol, 2-methylbutan-3-ol and 2,2-dimethylpropanol.

   Correlate the computationally obtained values of the dipole moments with the experimental values of the boiling points: (118 ºC, 100 ºC, 108 ºC, 82 ºC, of 1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2- propanol respectively).

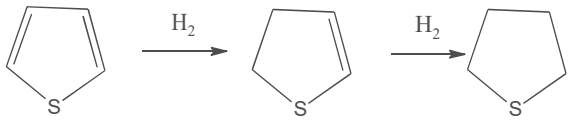
5) Based on the implicit electronic structure calculations, determine the heat of hydrogenation of Propylene.

6) Based on the calculations of enthanlies of the participating chemical species on optimized geometry of the molecules, calculate the reaction enthalpy at 298 K for the following, industrially important reactions:

   $$CH_4 + H_2O \rightarrow CO + 3H_2$$ (steam reforming of methane)

   ≡≡ (Haber-Bosch process)

7) Carry out geometry optimisation and determine the energy of the participating chemical species in the following reactions Using these results calculate the resonance energy of thiophene.



8) Carry out geometry optimisation & Energy calculations on the following species and obtain Frontier Molecular Orbitals. Visualize the Molecular Orbitals of these species and interpret the results for bonding in these molecules.
Benzene, Naphthalene, and Anthracene.

9) 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, $(CH_3)_2NH$, $(CH_3)_3N$

10) On the basis of results of geometry optimization and energy calculations, determine the enthalpy of isomerization of cis and trans 2-butene.

11) Perform a conformational analysis of butane. Plot the graph between the angle of rotation and the energy of the conformers using spreadsheet software.

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

13) Calculate the electronic UV/Visible absorption spectrum of Benzene.

14) Calculate the electronic absorption spectra of formaldehyde.

15) 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.

16) On a given set of molecules methylamine (CH_3NH_2) carry out geometry optimization, single point energy and NBO calculations and interpret the output results treated at the ab initio RHF/3-21G level.

17) Study the mechanism of SN_2 reaction between Cl^- and CH_3Br involving a Walden inversion computationally.

18) Perform a geometry optimization followed by a frequency assessment (opt+freq keyword) using the B3LYP method and 6-31-G(d) basis set on a given set of small molecules i.e. BH_3, CH_4.
Suggestive: A greater number of molecules may be studied as per instructions received from the concerned teacher.

19) Based on the fundamentals of conceptual DFT calculate the ionization potential (IP), electron affinity (EA), electronegativity and electron chemical potential of a given set of molecules.

20) Perform molecular docking of Sulfonamide-type D-Glucose inhibitor into MurrD active site using Argus Lab.

21) Perform molecular dynamics (MD) simulation of a given alkali metal ion in aqueous function (RDF)

Essential/recommended readings

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.
5. House, J.E. (2004), **Fundamentals of Quantum Chemistry**, 2nd Edition, Elsevier.
6. McQuarrie, D.A. (2016), **Quantum Chemistry**, Viva Books.
7. Levine, I. N.; **Physical Chemistry**, 5th Edition, McGraw –Hill.

Practical:

1. https://www.afs.enea.it/software/orca/orca_manual_4_2_1.pdf
2. https://dasher.wustl.edu/chem430/software/avogadro/learning-avogadro.pdf
3. http://www.arguslab.com/arguslab.com/ArgusLab.html
4. https://barrett-group.mcgill.ca/tutorials/Gaussian%20tutorial.pdf
5. https://gaussian.com/techsupport/
6. https://gaussian.com/man/
7. https://gaussian.com/wp-content/uploads/dl/gv6.pdf
8. https://dasher.wustl.edu/chem478/software/spartan-manual.pdf
9. http://www.mdtutorials.com/gmx/
10. https://vina.scripps.edu/manual/

Important Instruction Note on working approach:

- A student is required to perform/investigate a minimum of 10 exercises from the given set of exercises.
- The students may use open source softwares; ArgusLab, Avogadro and ORCA. In case a licenced version softwares is available, if procured by the college, other licenced softwares may also be used.

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