GENERIC ELECTIVES 17: CHEMISTRY: MOLECULAR MODELLING, ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING

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
		Lecture	Tutorial	Practical/ Practice		
Chemistry: Molecular Modelling, Artificial Intelligence and Machine Learning (GE-14)	4	2	0	2	Class XII Pass	----

Learning Objectives

- To make students familiar with modernscientific machine (programming) language i.e., Python, Artificial Intelligence (AI) & Machine Learning (ML) and their potential applications in chemistry.
- To provide elementary ideas of the techniques prevailing in the field of AI and ML and their applications to research problems especially related to research and development of new materials and pharmaceutical compounds with desired properties.

Learning outcomes

By the end of the course, the students will be:

- Conversant with the Python Programming Language.
- Familiar with Elementary techniques of AI and ML
- Able to apply techniques of AI & ML in basic problems of research in some important areas of research in Chemistry.

Syllabus Theory:

Part A: Molecular Modelling

Introduction to computational chemistry: **7 Hours**

Overview of Computational Methods in Chemistry (Ab initio, DFT, Semi- empirical, Molecular Mechanics

Potential Energy Surfaces **4 Hours**

The concept of Potential energy surface, Intrinsic Reaction Coordinates, Stationary points,

Equilibrium points – Local and Global minima, Geometry optimization and energy minimization.

Molecular Mechanics **4 Hours**

Force Fields (A brief idea of a basic force field), Elementary idea of MM1, MM2, MM3, MM4, MM+, AMBER etc. A brief Idea of Molecular Docking

Part B: Artificial Intelligence & Machine learning in Chemistry **15 Hours**

An overview of computationally readable and processible representation of molecules, e.g., SMILES, mol files. Chemical space and access to chemical databases. Statistical treatment of data: regression analysis andtypes of regression. Elementary Idea of Quantitative structure-activity relationship (QSAR).

An insight into Artificial Intelligence & Machine learning and potentialareas of applications in chemistry. Dimensional reduction; Principal Component Analysis (PCA) and the importance and necessity of nonlinearity in Artificial Intelligence.

Genetic algorithm, basics of random mutation hill climbing (RMHC) and simulated annealing.

Practicals: **(60 hours)**

Molecular Modeling based Exercise

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

2) Carry out geometry optimisation on H_2O, H_2S, H_2Se molecules and 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 mechanicalmethods.

3) Calculate the energy of the following chemical species andarrange 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 the geometry optimisation on the following chemical species and compare the shapes and dipole moments of the molecules.

1-butanol, 2-butanol, 2-methyl-1-propanol, and 2-methyl-2- propanol.

Correlate the computationally obtained values of the dipolemoments with the experimental values of the boiling points: (118ºC, 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 Ethene.

6) Based on the calculations of enthalpies 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)

$N_2 + 3\ H_2 \rightarrow 2NH_3$ (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 optimization & 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:
10) On the basis of results of geometry optimization and energy calculations, determine the enthalpy of isomerization of cis andtrans 2-butene.
11) QSAR based exercise on problems of interest to chemist.
12) Perform a conformational analysis of butane. Plot the graph between the angle of rotation and the energy of the conformers using spreadsheet software.
13) Compute the resonance energy of benzene by comparison of its enthalpy of hydrogenation with that of cyclohexene.
14) 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.

15) 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.
16) Perform molecular docking of Sulfonamide-type D-Glu inhibitor into MurD active site using Argus lab.

Artificial Intelligence (AI) and Machine Learning (ML) based exercise on problems of interest to chemist

17. Travelling salesman problem and electrical circuit design (minimization of path-length).
18. Genetic algorithm, in solving matrix form of linear equations
19. Non-linear least-square fitting problem.
20. Particle Swarm Optimization on the sphere function.

Important Instruction Note on working approach:

- A student is required to perform/investigate a minimum of 10 exercises in total.
- The exercises mentioned above will be performed by the student strictly in accordance with the instructions received and only under the supervision of the teacher concerned.
- Any other exercise may be carried out with prior permission, input, discussion and instructions received from the teacher concerned.

References:

1. Lewars, E. (2003), **Computational Chemistry**, Kluwer academicPublisher.
2. Cramer, C.J. (2004), **Essentials of Computational Chemistry**, John Wiley & Sons.
3. Cartwright C.; Kharma N., (2008), **Using artificial intelligence in chemistry and biology**, First Edition, CRC Press Taylor & Francis Group
4. Hippe; Z., **Artificial Intelligence in Chemistry: Structure Elucidation and Simulation of Organic Reactions**, (1991) Academic Press, Elsevier
5. Soft Computing in Chemical and Physical Sciences A Shift in Computing Paradigm (Kanchan Sarkar, Sankar Prasad Bhattacharyya) (z-lib.org)
6. Understanding Properties of Atoms, Molecules and Materials (PRANAB. SARKAR, Sankar Prasad Bhattacharyya) (z-lib.org)

Web Resources:

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/

Teaching Learning Process: Hands-on laboratory exercises Conventional teaching learning method. Engaging students in collaborative learning

Keywords: Molecular Modeling, Potential Energy Surface (PES), Geometry Optimization, Frequency calculation, Artificial Intelligence, Machine Learning, Nural Networks, Genetic Algorithm.

Note: Examination scheme and mode shall be as prescribed by the Examination Branch, University of Delhi, from time to time.