DISCIPLINE SPECIFIC ELECTIVE COURSE - 22 (DSE-22): Machine Learning and Artificial Intelligence in Chemistry

***For syllabus content of Discipline Specific Elective-22: (DSE-22)** "Machine Learning and Artificial Intelligence in Chemistry refer to the pool of DSE courses in 4th year syllabus of **B.Sc. (H) Chemistry**.

DISCIPLINE SPECIFIC ELECTIVE COURSE-VI (DSE-VI):

Title: Machine Learning and Artificial Intelligence in Chemistry (DSE-VI, Semester-VIII, 30 Lectures)

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course (if any)
		Lecture	Tutorial	Practical/ Practice		
Machine Learning and Artificial Intelligence in Chemistry (DSE-VI, Semester-VIII, 30 Lectures)	04	02	---	02	Class 12th with Physics, Chemistry, Mathematics	---

Course Objectives

- To develop a fundamental understanding of ML/AI, including their basic concepts and different types of learning
- To become familiar with the basic mathematical foundations of ML
- To understand the principles of ML/AI as applied to chemistry.
- To explore the applications of ML/AI in molecular modeling, drug discovery, quantum-mechanical calculations, catalysis, materials design, etc.
- To gain hands-on experience in implementing ML/AI algorithms and tools in solving chemical problems.

Learning Outcome

After completion of this course, learners will be able to-

- Understand core ML/AI principles, including data preprocessing, model training, evaluation, and types of learning.
- Implement and assess ML/AI models (regression, classification, neural networks) for chemistry problems.
- Apply ML/AI to chemical tasks like property prediction, reaction mechanisms, and spectroscopy.
- Integrate ML/AI with quantum chemistry to improve computational efficiency.

Course Contents (Theory) **Credit: 2 (30 lectures)**

Unit I: Introduction to ML/AI in Chemistry (6 lectures)
Overview of Machine Learning (ML) and Artificial Intelligence (AI). Data pre-processing, model selection, training, and evaluation. Types of learning: Supervised and unsupervised learning. Chemistry-specific challenges in applying AI/ML.
Unit II: Mathematics for ML/AI (6 lectures)
Linear Algebra: Vector and Matrix Dot Product, Probability Theory: Random Variables, Bayes Theorem, Conditional Probability, Optimisation: Gradient Descent, First/Second Order Condition.
Unit III: Machine Learning Models and Techniques (8 lectures)
Regression and classification models (Linear Regression, SVMs, Decision Trees), Kernel Ridge regression, Neural networks and deep learning, Backpropagation (qualitative), Unsupervised methods: Clustering.
Unit IV: Applications of ML/AI in Chemistry (10 lectures)
Application of ML/AI for the discovery of Molecular Design, Materials Sciences and Computational Chemistry; Predicting molecular properties. Prediction of reaction mechanisms and pathways. Binding affinity prediction and molecular docking. QSAR modelling in drug discovery, ML/AI in the design of functional materials and pharmaceutical chemistry. Predicting spectroscopic properties (IR, NMR, Raman). Accelerating quantum chemistry with ML/AI (e.g., approximating post-HF methods, PES fitting).

Recommended Texts/References:

1) Hugh M Cartwright (Ed), Machine Learning in Chemistry: The Impact of Artificial Intelligence, Royal Society of Chemistry; 1st edition (2020)
2) Jon Paul Janet, Heather J. Kulik, Machine Learning in Chemistry, American Chemical Society (2020)
3) Hugh M. Cartwright Applications of Artificial Intelligence in Chemistry, Oxford Chemistry Primers (1994)
4) Pavlo O. Dral, Quantum Chemistry in the Age of Machine Learning, Elsevier - Health Sciences Division (2022)
5) Artificial Intelligence in Chemistry: Current Trends and Future Directions, *J. Chem. Inf. Model.* 2021, 61, 3197−3212
6) A Gentle Introduction to Machine Learning for Chemists: An Undergraduate Workshop Using Python Notebooks for Visualization, Data Processing, Analysis, and Modelling, *J. Chem. Educ.* 2021, 98, 9, 2892–2898
7) The Dawn of Generative Artificial Intelligence in Chemistry Education, *J. Chem. Educ.* 2024, 101, 2957−2959
8) Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems, *Chem. Rev*. 2021, 121, 9816−9872
9) Current and Future Roles of Artificial Intelligence in Medicinal Chemistry Synthesis, *J. Med. Chem.* 2020, 63, 8667−8682
10) Artificial Chemical Intelligence: AI for Chemistry and Chemistry for AI by Prof. Pratyush Tiwary, Link: https://www.youtube.com/watch?v=B3wn3C2ANUw

Laboratory Exercises (at least 10 practical) **Credit: 2**

1) Fit a polynomial curve using Excel/spreadsheets/colab (linear, quadratic, cubic, quartic, etc) to find a trendline.
2) Perform interpolation and extrapolation on chemical datasets and also find the missing data.
3) Examine extrapolation to predict future values or trends.
4) Build and train a neural network model for molecular property prediction.
5) Running a simple neural network model in machine learning.

6) Fit potential energy surfaces (PES) using neural networks.
7) Use regression models on open-source chemical data (e.g., QM9).
8) Train regression models to predict spectra from structural data.
9) ML pipeline creation in scikit-learn using simple property prediction.
10) Use standard ML python pipelines to train models.
11) Visualization & analysis using tools like Jupyter notebooks/Google Colab.
12) Explore tools and libraries like Numpy, scikit-learn, PyTorch etc. for chemistry research, education, and data analysis.
13) Optional: Explore AI-driven retrosynthesis using IBM RXN or similar platforms (demo only).

References:

1. A Gentle Introduction to Machine Learning for Chemists: An Undergraduate Workshop Using Python Notebooks for Visualization, Data Processing, Analysis, and Modeling, *J. Chem. Educ.* 2021, 98, 9, 2892–2898
2. The Dawn of Generative Artificial Intelligence in Chemistry Education, *J. Chem. Educ.* 2024, 101, 2957−2959
3. Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems, *Chem. Rev*. 2021, 121, 9816−9872
4. McQuarrie & Simon**,** *Physical Chemistry: A Molecular Approach* (for PES concept)
5. a) https://jupyter.org/ b) https://colab.research.google.com/ c) https://www.python.org/ d) https://numpy.org/ e) https://scikit-learn.org/stable/ f) https://pytorch.org/

List of Instruments/Software required for Fourth year for each College

1. UV- Vis Spectrophotometer
2. Digital Photo Fluorometer
3. Polarimeter
4. Table top IR Spectrophotometer
5. ChemDraw
6. HyperChem
7. Access to NMR Spectrophotometer in Department of Chemistry/USIC
8. Rota Evaporator