

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