

Details of Course

Course Title	Course Structure			Pre-Requisite
Artificial Intelligence for Material Science- B.Tech. EP IV Sem Lesson Plan	L	T	P	Students should have a foundational knowledge of programming and statistics.
	3	0	2	

Course Objectives

This course introduces AI and ML techniques and their applications in materials science. It covers the fundamentals of AI and ML, including supervised, unsupervised, and reinforcement learning, and explores their use in predicting material properties, discovering new materials, and optimizing materials for specific applications. The course includes a lab component where students will work on projects using AI tools and datasets to solve real-world materials science problems.

Course Outcomes (CO)

1. To understand the basic principles and algorithms of AI and ML.
2. To analyse different databases for material science applications.
3. To Apply AI and ML techniques to solve problems in materials science.
4. To evaluate the effectiveness of various AI models.
5. To use AI tools and software for materials design and analysis.

S. No.	Content	Contact Hours
Unit 1	Introduction to Artificial Intelligence: History, evolution, and significance in today's world. AI in Materials Science: Overview of potential applications and case studies demonstrating successful implementations. Basic Concepts of Machine Learning: Overview of supervised, unsupervised, and reinforcement learning with examples relevant to materials science.	8
Unit 2	Data Handling and Preprocessing Data Collection: Sources of data in materials science, including experimental, computational, and literature-derived datasets. Data Cleaning and Normalization: Techniques for dealing with missing data, outliers, and normalization of datasets to prepare them for analysis. Feature Engineering: Importance of domain knowledge in creating features that can significantly impact model performance.	8
Unit 3	Supervised Learning in Materials Science Regression Analysis: Techniques like linear regression, polynomial regression, and their applications in predicting quantitative material properties.	8

	Classification: Use of logistic regression, support vector machines, and decision trees for categorizing materials into predefined classes based on their properties or behaviours.	
Unit 4	Unsupervised Learning and Dimensionality Reduction Clustering Techniques: k-means clustering, hierarchical clustering, and their applications in grouping materials based on similarities in properties or compositions without labelled data. Dimensionality Reduction: Techniques such as Principal Component Analysis (PCA) and t-Distributed Stochastic Neighbour Embedding (t-SNE) to visualize high-dimensional data and identify underlying patterns.	8
Unit 5	Deep Learning for Materials Science Introduction to Neural Networks: Basics of neural networks, including their architecture, activation functions, and how they learn. Convolutional Neural Networks (CNNs): Application of CNNs in image-based analysis of materials, such as microstructure characterization and defect detection. Reinforcement Learning and its Applications Basics of Reinforcement Learning: Understanding the reinforcement learning paradigm and its components: agent, environment, states, actions, and rewards.	10
	Total	42

Books:

S. No.	Name of Books/Authors/Publisher
1.	“Introduction to Machine Learning” by Ethem Alpaydin (MIT Press, Prentice Hall of India, 3rd Edition 2014)
2.	“An introduction to Statistical Learning” with application in Python edited by Gareth James, Daniela Witten, Trevor, Trevor Hastie, Robert Tibshirani and Jonathan Taylor (Springer Texts in Statistics, second edition 2023)
	“Foundations of Machine Learning” by Mehryar Mohri, Afshin Rostamizadeh, Ameet Talwalkar (MIT Press, 2012).
3.	“Materials Informatics: Methods, Tools, and Applications” edited by Olexandr Isayev, Alexander Tropsha and Stefano Curtarolo (John Wiley & Sons, 2019)
4.	"Python for Data Analysis" by Wes McKinney.
5.	Artificial Intelligence for Material Science edited by Yuan Cheng, Tian Wang, Gang Zhang (Springer series in Material Science, Volume 312)
6.	Online resources and documentation for TensorFlow, PyTorch, and relevant AI and materials science databases.

List of the Experiments:

- Querying, Organizing and Visualizing Materials Data: Using Python libraries to clean, preprocess, and visualize materials science data.
 1. Query from Pymatgen (Processing and Organizing Data, Plotting)
 2. Query from Mendeleeev
 3. a) Find the three metals with highest Young's moduli.
b) What are the Young's moduli of Al, Fe and Pb.
- Building and Evaluating Regression Models: Implementing regression models to predict material properties.
 4. Getting data, processing, and organizing Data
 5. Creating the Model and Plotting
- Classification Models for Material Identification:
 6. Using supervised learning algorithms to classify materials based on their features.
- Clustering for Materials Discovery:
 7. Applying unsupervised learning techniques to discover new material groups.
- Using neural networks to predict and classify crystal structures of elements:
 8. Getting a dataset, processing, and organizing the data
 9. Creating the Model and Plotting
 10. Using neural networks to estimate Young's Modulus for elements.