MSE6186: AI FOR MATERIALS SCIENCE

Effective Term
Semester A 2026/27

Part I Course Overview

Course Title
AI for Materials Science

Subject Code
MSE - Materials Science and Engineering

Course Number
6186

Academic Unit
Materials Science and Engineering (MSE)

College/School
College of Engineering (EG)

Course Duration
One Semester

Credit Units
3

Level
P5, P6 - Postgraduate Degree

Medium of Instruction
English

Medium of Assessment
English

Prerequisites
Nil

Precursors
Nil

Equivalent Courses
Nil

Exclusive Courses
Nil

Part II Course Details

Abstract
The course emphasizes classical, interpretable models, practical data workflows, and hands-on problem solving. Weekly lectures and tutorials guide students through core concepts, including supervised and unsupervised learning, classification

and regression, and models such as k-nearest neighbors, linear and logistic regression, decision trees, random forests, clustering methods and so on. Students learn to prepare datasets, train and validate models, avoid overfitting, and interpret results critically. Tutorials focus on Python-based tools including NumPy, Pandas, Matplotlib, and scikit-learn. Assessments include assignments, quizzes, and a midterm exam. The course concludes in an in-class modelling challenge and a guest industry seminar highlighting real-world AI applications. By the end, students gain the ability to apply machine learning appropriately and evaluate its limitations in scientific and engineering contexts.

Course Intended Learning Outcomes (CILOs)

	CILOs	Weighting (if app.)	DEC-A1	DEC-A2	DEC-A3
1	Recognize the role and scope of machine learning in scientific and engineering contexts, particularly within materials science.	10	x		
2	Demonstrate the application of classical machine learning models (e.g., kNN, linear/logistic regression, decision trees) to representative data-driven problems.	20		x	
3	Identify key factors affecting model performance and reliability, including data quality, feature selection, validation strategies, and overfitting.	20	x		
4	Evaluate modern developments in machine learning and AI tools to form critical perspectives and support independent problem-solving.	20		x	
5	Apply Python-based machine learning workflows (NumPy, Pandas, scikit-learn) to solve structured problems in materials science, physics, chemistry, and related fields.	30			x

A1: Attitude
Develop an attitude of discovery/innovation/creativity, as demonstrated by students possessing a strong sense of curiosity, asking questions actively, challenging assumptions or engaging in inquiry together with teachers.

A2: Ability
Develop the ability/skill needed to discover/innovate/create, as demonstrated by students possessing critical thinking skills to assess ideas, acquiring research skills, synthesizing knowledge across disciplines or applying academic knowledge to real-life problems.

A3: Accomplishments
Demonstrate accomplishment of discovery/innovation/creativity through producing /constructing creative works/new artefacts, effective solutions to real-life problems or new processes.

Learning and Teaching Activities (LTAs)

	LTAs	Brief Description	CILO No.	Hours/week (if applicable)
1	Lectures	Lectures	1, 2, 3, 4	1.5 hrs/wk
2	Tutorials	Tutorials	2, 3, 4, 5	1 hr/wk
3	Project	Project	5	0.5 hrs/wk

Assessment Tasks / Activities (ATs)

	ATs	CILO No.	Weighting (%)	Remarks ("-" for nil entry)	Allow Use of GenAI?
1	Assignments	1, 2, 3, 4, 5	35	performance assessment purpose	Yes
2	Project	5	30	Inc. project report and presentation	Yes
3	Mid-term Test	1, 2, 3, 4, 5	35	-	No

Continuous Assessment (%)

100

Assessment Rubrics (AR)

Assessment Task

Assignments (Applicable to students admitted before Semester A 2022/23 and in Semester A 2024/25 & thereafter)

Criterion

The student successfully completes all assessment tasks, demonstrating strong understanding of underlying machine learning principles, model architectures, and algorithmic mechanisms.

Excellent

(A+, A, A-) High

Good

(B+, B, B-) Significant

Fair

(C+, C, C-) Moderate

Marginal

(D) Basic

Failure

(F) Not reaching marginal level

Assessment Task

Mid-term Test (Applicable to students admitted before Semester A 2022/23 and in Semester A 2024/25 & thereafter)

Criterion

The student can accurately identify, interpret, and explain how machine learning principles are applied to scientific and technological problems, particularly within materials science contexts.

Excellent

(A+, A, A-) High

Good

(B+, B, B-) Significant

Fair

(C+, C, C-) Moderate

Marginal

(D) Basic

Failure
(F) Not reaching marginal level

Assessment Task
Project (Applicable to students admitted before Semester A 2022/23 and in Semester A 2024/25 & thereafter)

Criterion
The student is able to design and implement a machine learning or simulation-based approach using course concepts to solve a scientific problem. The student can critically analyze results, draw meaningful conclusions, and communicate findings effectively through clear written reports and/or oral presentations.

Excellent
(A+, A, A-) High

Good
(B+, B, B-) Significant

Fair
(C+, C, C-) Moderate

Marginal
(D) Basic

Failure
(F) Not reaching marginal level

Assessment Task
Assignments (Applicable to students admitted from Semester A 2022/23 to Summer term 2024)

Criterion
The student successfully completes all assessment tasks, demonstrating strong understanding of underlying machine learning principles, model architectures, and algorithmic mechanisms.

Excellent
(A+, A, A-) High

Good
(B+, B) Moderate

Marginal
(B-, C+, C) Basic

Failure
(F) Not reaching marginal level

Assessment Task
Mid-term Test (Applicable to students admitted from Semester A 2022/23 to Summer term 2024)

Criterion

The student can accurately identify, interpret, and explain how machine learning principles are applied to scientific and technological problems, particularly within materials science contexts.

Excellent

(A+, A, A-) High

Good

(B+, B) Moderate

Marginal

(B-, C+, C) Basic

Failure

(F) Not reaching marginal level

Assessment Task

Project (Applicable to students admitted from Semester A 2022/23 to Summer term 2024)

Criterion

The student is able to design and implement a machine learning or simulation-based approach using course concepts to solve a scientific problem. The student can critically analyze results, draw meaningful conclusions, and communicate findings effectively through clear written reports and/or oral presentations.

Excellent

(A+, A, A-) High

Good

(B+, B) Moderate

Marginal

(B-, C+, C) Basic

Failure

(F) Not reaching marginal level

Part III Other Information

Keyword Syllabus

· **Introduction**

Overview of machine learning in science and engineering. Role of data-driven modeling in materials science, physics, chemistry, and life science.

· **Probability Theory and Statistics**

Random variables and distributions. Expectation and variance. Conditional probability.

· **Linear Models**

Linear regression. Ridge and Lasso regularization. Logistic regression. Bias–variance trade-off. Model interpretability.

· **Classical Machine Learning Models**

k-Nearest Neighbors (kNN). Decision trees. Random forests. Support vector machines (SVM). Kernel methods. Ensemble learning (bagging, boosting).

· **Optimization Methods**

Loss functions. Gradient descent and stochastic gradient descent (SGD). Convex optimization. Regularization techniques. Hyperparameter tuning.

- **Neural Networks and Deep Learning (Introduction)**

Perceptron. Multi-layer neural networks. Backpropagation. Activation functions. Overfitting and regularization.

- **Unsupervised Learning**

Clustering (k-means, hierarchical clustering). Dimensionality reduction (PCA). Feature extraction and representation learning.

- **Model Evaluation and Validation**

Training, validation, and test sets. Cross-validation. Performance metrics (MSE, R^2, accuracy, precision, recall). Model selection.

- **Scientific Applications of Machine Learning**

Applications in materials discovery, molecular modeling, biophysics, and chemical systems. Integration with simulation methods (e.g., molecular dynamics).

- **Project**

A discovery-oriented multidisciplinary project applying machine learning to scientific problems such as materials design, molecular systems, or biological data, including model development, analysis, and presentation.

Reading List

Compulsory Readings

	Title
1	https://scikit-learn.org/stable/supervised_learning.html
2	https://scikit-learn.org/stable/modules/clustering.html
3	https://scikit-learn.org/stable/modules/decomposition.html
4	https://scikit-learn.org/stable/model_selection.html
5	https://scikit-learn.org/stable/modules/preprocessing.html

Additional Readings

	Title
1	Machine Learning A Probabilistic Perspective – Kevin P. Murphy. In-depth probabilistic framework covering modern machine learning approaches and inference techniques.
2	Hands-On Machine Learning with Scikit-Learn Keras and TensorFlow – Aurélien Géron. Practical guide to implementing machine learning models, useful for project-based learning.
3	Pattern Recognition and Machine Learning – Christopher M. Bishop.
4	The Elements of Statistical Learning – Trevor Hastie, Robert Tibshirani, and Jerome Friedman.
5	Deep Learning – Ian Goodfellow, Yoshua Bengio, and Aaron Courville. Standard reference for neural networks and deep learning fundamentals.