

DSC6025: AI FOR MATERIALS SCIENCE

Effective Term

Semester A 2026/27

Part I Course Overview

Course Title

AI for Materials Science

Subject Code

DSC - Data Science

Course Number

6025

Academic Unit

Data Science (DS)

College/School

College of Computing (CC)

Course Duration

One Semester

Credit Units

3

Level

P5, P6 - Postgraduate Degree

Medium of Instruction

English

Medium of Assessment

English

Prerequisites

Fundamental knowledge of materials science; Calculus; Linear algebra; Basic knowledge in Python.

Precursors

Nil

Equivalent Courses

SDSC6025 AI for Materials Science

Exclusive Courses

Nil

Part II Course Details

Abstract

This teaching plan offers a structured exploration of artificial intelligence (AI) applications in materials science, with adaptable content depth tailored to various expertise levels. It encompasses introductory lectures on AI relevance in

materials science, progressing to data science fundamentals and hands-on activities. The curriculum includes AI tools, supervised and unsupervised learning techniques, and data-driven optimization strategies applicable to materials science. Key topics such as Convolutional Neural Networks, boosting algorithms, dimensionality reduction techniques, and Bayesian optimization are covered in depth. 3-month timetable details weekly sessions, including lectures, practical exercises, and assignments to reinforce learning. Students will engage in hands-on projects to apply AI techniques to real-world materials science problems, culminating in a comprehensive exam and final project. The plan emphasizes collaborative learning and flexibility to accommodate varying student backgrounds.

Course Intended Learning Outcomes (CILOs)

CILOs		Weighting (if DEC-A1 app.)		DEC-A2	DEC-A3
1	Mastering the concept of artificial intelligence and its application in materials science	25	x		
2	Ability to program in python and relevant AI code	25	x		
3	Apply data-driven tools to materials science problems	25		x	
4	Discuss state-of-the-art development in the relevant areas and to form opinions on specific issues.	25			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		1, 2, 3, 4	25 hours/sem
2	Tutorials		1, 2, 3, 4	6 hours/sem
3	Assignments		1, 2, 3	8 hours/sem

Assessment Tasks / Activities (ATs)

ATs		CILO No.	Weighting (%)	Remarks ("-" for nil entry)	Allow Use of GenAI?
1	Assignments	2, 3, 4	60	-	Yes

Continuous Assessment (%)

60

Examination (%)

40

Examination Duration (Hours)

2

Minimum Examination Passing Requirement (%)

30

Assessment Rubrics (AR)

Assessment Task

Assignments (for students admitted in Semester A 2026/27 & thereafter)

Criterion

Train students' ability to theorize and solve various types of AI for materials science problems.

Excellent

(A+, A, A-) High

Good

(B+, B, B-) Significant

Fair

(C+, C, C-) Moderate

Marginal

(D) Basic

Failure

(F) Not even reaching marginal levels

Assessment Task

Examination (for students admitted in Semester A 2026/27 & thereafter)

Criterion

It assesses students' ability to theorize and solve various types of AI for materials problems.

Excellent

(A+, A, A-) High

Good

(B+, B, B-) Significant

Fair

(C+, C, C-) Moderate

Marginal

(D) Basic

Failure

(F) Not even reaching marginal levels

Part III Other Information

Reading List

Additional Readings

Title	
1	Ian Goodfellow and Yoshua Bengio and Aaron Courville. Deep Learning. 2016. ISBN: 978-0262035613.
2	Charles Audet and Warren Hare. Derivative-Free and Blackbox Optimization. 2017. ISBN: 978-3319689128
3	Laura Igual , Santi Seguí. Introduction to Data Science. 2024. ISBN: 978-3031489556