

	MScNano W-MMC
Code	Machine Learning for Materials and Chemistry
Module type	Wahlpflichtmodul / Required elective module
Educational outcomes, competencies, qualification objectives	<p>Studierende</p> <ul style="list-style-type: none"> - haben einen Einblick in modernes maschinelles Lernen für Anwendungen in Materialwissenschaften und Chemie - können Methoden des maschinellen Lernens selbständig auf Forschungsfragen anwenden/implementieren - sind in der Lage, Spezialliteratur des angewandten maschinellen Lernens zu lesen und sie einem fortgeschrittenen Publikum zu präsentieren <p>Students</p> <ul style="list-style-type: none"> ... have insight into modern machine learning for applications in materials science and chemistry ... are able to apply/implement machine learning methods to research questions ... are able to read special research literature in applied machine learning and present it to an advanced audience
Types of courses, contact hours	VL 2 SWS Ü 2 SWS
Contents	<p>Lecture:</p> <ul style="list-style-type: none"> - Data sets and problem categories - Mapping practical problems in materials and chemistry to machine learning applications - Regression - Classification - Clustering - Deep Learning - Kernel Methods - Derivatives in chemical space - Representations for molecules and materials - Training procedures and hyperparameter optimization <p>Exercise:</p> <ul style="list-style-type: none"> - Brief introduction in the scripting language Python. - Implementation of Machine Learning models in Python - Practical application of to design problems of materials science or Chemistry
Course titles	Machine Learning for Materials and Chemistry (VL), Applied Machine Learning for Materials and Chemistry (Ü)
Teaching methods	Lecture, exercises
Applicability	
Duration	one semester
Frequency	anually
Language	English
Recommended Skills	Fundamental knowledge in physics or chemistry on Bachelor level
Prerequisites for participation	None
Students workload	150 h (Kontaktzeit 60 h, Selbststudium 90 h) (Contact time: 60 h, Independent studies: 90 h)
Course projects / nongraded learning assignments (Studienleistungen)	Successful participation at exercises
Prerequisites for admission to examination	None
Examination	Klausur (1-2 h) oder mündliche Prüfung (30 min) written (1-2 h) or oral exam (30 min)
Number of credits	5 C
Lehreinheit	Chemie
Responsible coordinator	von Rudorff
Lecturer(s)	von Rudorff
Media	Slides, code sessions, videos
Literature	The updated literature will be announced in the lecture.