

## 课程详述

### COURSE SPECIFICATION

以下课程信息可能根据实际授课需要或在课程检讨之后产生变动。如对课程有任何疑问，请联系授课教师。

The course information as follows may be subject to change, either during the session because of unforeseen circumstances, or following review of the course at the end of the session. Queries about the course should be directed to the course instructor.

1.	课程名称 Course Title	材料科学中的 AI 方法导论 Introduction to AI for Materials Science
2.	授课院系 Originating Department	材料科学与工程系 Department of Materials Science and Engineering
3.	课程编号 Course Code	MSE104
4.	课程学分 Credit Value	1
5.	课程类别 Course Type	通识选修课程 General Education (GE) Elective Courses
6.	授课学期 Semester	春季 Spring
7.	授课语言 Teaching Language	中文 Chinese
8.	授课教师、所属学系、联系方式 (如属团队授课, 请列明其他授课教师) Instructor(s), Affiliation & Contact (For team teaching, please list all instructors)	李保文, 讲席教授, 材料科学与工程系, libw@sustech.edu.cn Chair Prof. Baowen Li, MSE, libw@sustech.edu.cn 张文清, 教授, 材料科学与工程系, zhangwq@sustech.edu.cn Prof. Wenqing Zhang, MSE, zhangwq@sustech.edu.cn 刘玮书, 教授, 材料科学与工程系, liuws@sustech.edu.cn Prof. Weishu Liu, MSE, liuws@sustech.edu.cn 李磊, 副教授, 材料科学与工程系, lil33@sustech.edu.cn Associate Prof. Lei Li, MSE, lil33@sustech.edu.cn 罗光富, 助理教授, 材料科学与工程系, luogf@sustech.edu.cn Assistant Prof. Guangfu Luo, MSE, luogf@sustech.edu.cn 邬家臻, 助理教授, 材料科学与工程系, wujz@sustech.edu.cn Assistant Prof. Jiazhen Wu, MSE, wujz@sustech.edu.cn
9.	实验员/助教、所属学系、联系方式 Tutor/TA(s), Contact	待公布 To be announced
10.	选课人数限额(可不填) Maximum Enrolment (Optional)	

11. 授课方式 Delivery Method	讲授	习题/辅导/讨论	实验/实习	其它(请具体注明)	总学时
	Lectures	Tutorials	Lab/Practical	Other (Please specify)	Total
学时数 Credit Hours	8	8			16
12. 先修课程、其它学习要求 Pre-requisites or Other Academic Requirements	无 NA				
13. 后续课程、其它学习规划 Courses for which this course is a pre-requisite					
14. 其它要求修读本课程的学系 Cross-listing Dept.					

### 教学大纲及教学日历 SYLLABUS

#### 15. 教学目标 Course Objectives

本课程重点讲解大数据和人工智能方法在材料科学中的应用以及对科学研究范式的深刻改变。课程通过模块化方式进行教学，内容涵盖材料科学研究历史和研究方法的演化、Python 语言基础教学以及人工智能在材料科学中引人入胜的典型应用案例，如人工智能设计热学超材料。最终让学生亲身体会人工智能和材料科学相结合所产生的巨大影响，激发学生深入思考人工智能、大数据以及人工智能驱动的材料研究新方法。

This course serves as an introduction to the 'Artificial Intelligence in Materials Science' series. It is designed with a modular approach, teaching the research paradigm evolution of materials science, with focus on the fourth paradigm of big data and artificial intelligence. The course will cover the necessary Python knowledge and the case studies of AI for Materials Science. Through engaging case studies, such as the AI for the design of thermal meta-materials, which will let students to experience the spark between AI and materials science, and also have new thoughts on the AI, Big Data, and the emerging paradigm of AI-driven materials research.

Southern University  
of Science and  
Technology

#### 16. 预达学习成果 Learning Outcomes

本课程学习完成后，学生将初步理解机器学习方法及其在材料科学中的应用，熟悉该方法在加速材料性质模拟、发现新材料的工作流程，并能够利用诸如神经网络、决策树、图神经网络等典型机器学习方法预测材料性质。

Upon completing the 'Introduction to AI for Materials Science,' students will gain a brief understanding of machine-learning techniques and their relevance in the field of materials science. They will acquire knowledge of the fundamental workflow for employing machine-learning methods to expedite atomic simulations of materials and aid in the discovery of new materials. Additionally, they will be capable of applying common machine-learning methods, such as neural networks, decision trees, and graph neural networks, in the prediction of material properties.

#### 17. 课程内容及教学日历（如授课语言以英文为主，则课程内容介绍可以用英文；如团队教学或模块教学，教学日历须注明主讲人）

**Course Contents (in Parts/Chapters/Sections/Weeks. Please notify name of instructor for course section(s), if this is a team teaching or module course.)**

第一讲：材料科学简介：简要介绍新材料的研究历史及材料科学研究方法的演化（2学时）

**Lecture 1:** Introduction to materials science: a brief introduction to the history of discovery of new materials and

paradigm in materials research and development. (2 credit hours)

第二讲：机器学习方法及其应用简介：简要介绍从线性拟合到神经网络在内的多种机器学习方法在材料科学中的最新应用（2学时）

**Lecture 2:** Introduction to modern machine-learning methods and application examples: a brief introduction with cutting-edge examples in materials science, covering a spectrum of approaches from basic linear fitting and perceptrons to advanced techniques (neural network, decision trees, etc.). (2 credit hours)

第三讲：面向人工智能的 Python 语言编程：简要介绍数据类型、数据结构、循环、函数、利用外部库文件实现面向对象编程（2学时）

**Lecture 3:** Python programming fundamentals for AI: a concise overview of the subsequent subjects, including data types, compound data structures (lists, tuples, dictionaries), loops, functions and object-oriented programming with external libraries (examples with PyTorch). (2 credit hours)

第四讲：深度神经网络在原子尺度的应用：利用深度神经网络和简化模型模拟材料中的原子运动（2学时）

**Lecture 4:** Sculpting the atomic world with deep neural network: explore the application of deep neural networks in simulating movements of atoms within materials through a simple toy model. (2 credit hours)

第五讲：人工智能辅助设计热学超材料（2学时）

**Lecture 5:** AI-assisted design of thermal meta-materials. (2 credit hours)

第六讲：人工智能辅助设计热电材料（2学时）

**Lecture 6:** AI-assisted design of thermoelectric materials. (2 credit hours)

第七讲：人工智能辅助设计力学超材料（2学时）

**Lecture 7:** AI-assisted design of mechanical meta-materials. (2 credit hours)

第八讲：人工智能辅助材料制备（2学时）

**Lecture 8:** AI application in materials fabrication. (2 credit hours)



**18. 教材及其它参考资料 Textbook and Supplementary Readings**

无/NA

**课程评估 ASSESSMENT**

19. 评估形式 Type of Assessment	评估时间 Time	占考试总成绩百分比 % of final score	违纪处罚 Penalty	备注 Notes
出勤 Attendance		20		
课堂表现 Class Performance				
小测验 Quiz				
课程项目 Projects				
平时作业 Assignments				
期中考试				

<b>Mid-Term Test</b>				
期末考试 <b>Final Exam</b>				
期末报告 <b>Final Presentation</b>		80		
其它（可根据需要 改写以上评估方式） <b>Others (The above may be modified as necessary)</b>				

20. 记分方式 **GRADING SYSTEM**

- A. 十三级等级制 **Letter Grading**  
 B. 二级记分制（通过/不通过） **Pass/Fail Grading**

**课程审批 REVIEW AND APPROVAL**

21. 本课程设置已经过以下责任人/委员会审议通过  
**This Course has been approved by the following person or committee of authority**