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**	计算材料学 Computational 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**	MSE343
4.	**课程学分 Credit Value**	3
5.	**课程类别 Course Type**	专业选修课 Major-Elective Course
6.	**授课学期 Semester**	春季 Spring semester
7.	**授课语言 Teaching Language**	中英双语 English & 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）**	罗光富 材料科学与工程系 luogf@sustech.edu.cn Guangfu Luo Department of Materials Science and Engineering luogf@sustech.edu.cn
9.	**实验员/助教、所属学系、联系方式 Tutor/TA(s), Contact**	
10.	**选课人数限额(可不填) Maximum Enrolment （Optional）**	

11. 授课方式 Delivery Method	讲授 Lectures	习题/辅导/讨论 Tutorials	实验/实习 Lab/Practical	其它(请具体注明) Other（Please specify）	总学时 Total
学时数 Credit Hours	30	4	30		64

12. 先修课程、其它学习要求 Pre-requisites or Other Academic Requirements	MSE203 晶体学 Crystallography
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

本课程针对有一定材料或固体物理基础的本科生和研究生。本课程将系统介绍计算材料科学中的密度泛函理论、分子动力学、多体量子力学方法的原理和适用范围，并通过使用前沿的科学计算软件和上机实习让学生去体验这些方法在半导体电子学、太阳能电池、锂离子电池、材料生长等领域的具体应用。

This course is designed for undergraduate and graduate students with knowledge of materials science or solid-state physics. It will introduce the fundamental theories and applications of three major methods used in Computational Materials Science: the Density Functional Theory, Molecular Dynamics, and Many-body Quantum Theory. Students will be given opportunities to learn the cutting-edge software and hands-on practices to experience the applications of these methods in the study of semiconductor electronics, solar cells, lithium-ion battery, and materials growth, etc.

16. 预达学习成果 Learning Outcomes

完成相关学习后，学生将对计算材料科学的重要性、主要研究方法、适用范围有基本认识。学会利用目前主流的科学计算软件去解决多个研究领域中的实际问题。

After this course, the students will understand the significance of Computational Materials Science, the major theories and tools, and their applications. Students will understand the procedures of utilizing cutting-edge software to address the relevant scientific issues in several research fields.

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.)

计算材料科学概述—Overview of Computational Materials Science（4 Credit Hours）
This section introduces the unique role of Computational Materials Science in nowadays scientific researches. Several scientific concepts and computational tools that go through the whole course will be introduced.

密度泛函基础—Fundamentals of Density Functional Theory（20 Credit Hours）
This section introduces the Density Functional Theory, covering its history, comparison with other methods, major capabilities/limitations, and critical settings/parameters to obtain reliable structural, electronic, optical, thermodynamical, and dynamical results.

密度泛函方法上机练习—Hands-on practice using Density Functional Theory（12 Credit Hours）
Students will utilize the VASP code to perform convergence tests, and to calculate and analyse total energy, structure, band structure, elastic modulus, piezoelectricity, IR/Raman spectrum, phonon spectrum, and activation barrier in several fields.

分子动力学基础—Introduction to Molecular Dynamics（4 Credit Hours）

This section will introduce the basic ideas of molecular dynamics, covering both the classic and *ab-initio* molecular dynamics.

分子动力学方法上机练习—Hands-on practice using Molecular Dynamics（8 Credit Hours）
Students will utilize the VASP and LAMMPS codes to study dynamical processes occurring in bulks and on film surfaces.

多体量子力学方法简介—Introduction to Many-body Quantum Theory（8 Credit Hours）
This section will introduce the GW and BSE methods, which can overcome the well-known limitations of the Density Functional Theory.

多体量子力学方法上机练习—Hands-on practice using Many-body Quantum Theory（8 Credit Hours）
Students will utilize the GW and BSE methods as implemented in the VASP and BerkeleyGW codes to obtain reliable band structure and optical properties.

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

Introduction to Solid State Physics, Charles Kittel, JOHN WILEY & SONS, 1956
Density Functional Theory: A Practical Introduction, David Sholl, Janice A Steckel, John Wiley and Sons Ltd,2009

Materials Modelling using Density Functional Theory: Properties and Prediction, Feliciano Giustino, Oxford University Press, USA,1988

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		15		
课堂表现 Class Performance		0		
小测验 Quiz		0		
课程项目 Projects		0		
平时作业 Assignments		55		
期中考试 Mid-Term Test		0		
期末考试 Final Exam		0		
期末报告 Final Presentation		30		Work on group project
其它（可根据需要改写以上评估方式） Others (The above may be modified as necessary)		0		

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