上海交通大学研究生专业课程信息收集表

Information Form for SJTU Graduate Profession Courses

<table>
<tr><th colspan="6">课程基本信息 Basic Information</th></tr>
<tr><td>*课程名称
Course Name</td><td colspan="5">（中文 Chinese）多尺度材料模拟与计算
（英文 English）Multiscale Materials Modeling and Simulation</td></tr>
<tr><td>*学分
Credits</td><td>3</td><td>*学时
Teaching Hours</td><td colspan="3">48（1 学分=16 课时）</td></tr>
<tr><td>*开课学期
Semester</td><td>秋季学期 Fall</td><td>*是否跨学期
Cross-semester?</td><td>否 No</td><td colspan="2">跨 Spanning over 个学期 Semesters（含夏季学期）。</td></tr>
<tr><td>*课程类型
Course Type</td><td>专业基础课 Program Core Course</td><td>*课程分类
Course Type</td><td colspan="3">全日制课程 For full-time students</td></tr>
<tr><td>*课程性质
Course Category</td><td>专业课 Specialized Course</td><td>课程层次
Targeting Students</td><td colspan="3">硕博共用 All graduates</td></tr>
<tr><td>*授课语言
Instruction Language</td><td>英文 English</td><td>主要授课方式
Teaching Method</td><td colspan="3">课堂教学 In class teaching</td></tr>
<tr><td>*成绩类型
Grade</td><td>等第制 Letter grading</td><td>主要考核方式
Exam Method</td><td colspan="3">操作 Hand-on</td></tr>
<tr><td>*开课院系
School</td><td colspan="5">材料科学与工程学院</td></tr>
<tr><td>所属学科
Subject</td><td colspan="5">材料科学与工程</td></tr>
<tr><td rowspan="2">负责教师
Person in charge</td><td>姓名 Name</td><td>工号 ID</td><td>单位 School</td><td colspan="2">联系方式 E-mail</td></tr>
<tr><td>孔令体</td><td></td><td>材料科学与工程学院</td><td colspan="2">konglt@sjtu.edu.cn</td></tr>
<tr><th colspan="6">课程扩展信息 Extended Information</th></tr>
<tr><td>*课程简介
(中文)
Course Description</td><td colspan="5">（分段概述课程定位、教学目标、主要教学内容、先修课程等；不少于 200 字。）
本课程是对材料科学与工程学科研究生的专业基础课，旨在培养学生材料科学计算的理念、概念与技能。主要讲授材料科学问题中跨尺度模拟与计算的概念与方法，着重介绍采用电子层次的第一性原理计算、原子及分子尺度的分子动力学模拟等方法的基本概念、基本原理、基本方法和典型应用，简要介绍介观、宏观尺度模拟方法，以及跨尺度模拟与计算、高通量计算与材料基因组的概念，使学生较为系统地掌握多尺度材料模拟与计算的基本概念和技能，深化对材料“结构-性能”本构关系的理解，激发并拓宽学生的材料研究理念与思维模式，使其能够运用新方法解决材料科学中的多尺度问题。本课程的实验教学内容涵盖数值模拟、统计分析、数据可视化等相关技术，并将介绍各尺度模拟计算的常用软件及可视化软件。</td></tr>
<tr><td>*课程简介
（English）
Course Description</td><td colspan="5">（须与中文一致，翻译请力求信达雅。）
As a program core course for materials science and engineering, this course aims to introduce the basic ideas, concepts, and techniques of materials modelling and simulation to the graduate students. This main contents of this course covers the basic concepts and methods for modeling and simulations of multiscale problems in materials science, with an emphasis on the basic concepts, theories, algorithms, and applications of electronic scale first-principles and atomic scale approaches such as molecular dynamics. Besides, the fundamental concepts of the mesoscale and macroscale methods will also be discussed, as well as the cross-scale methods, high-throughput calculations, and materials genome. It is expected that the student will gain some systematic knowledge on the ideas and skills for multiscale materials modeling and simulation, and in turn deepen their understanding on the constitutive relations between the structures and the properties of materials. The course also features some hand-on experiments which cover numerical simulations, statistical analysis, as well as visualization of the models/results. The main-stream software will also be introduced and used.</td></tr>
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*教学大纲
(中文)
Syllabus

（建议列表形式，各列内容：章节、主要内容、课时数、教学方式等）

教学内容 Content	授课学时 Hours	教学方式 Format
Introduction: scientific computation and scientific programming	3	Lecture
Molecular Dynamics methods: principles, algorithm, implementation, codes	3	Lecture
Interatomic potentials: theory, derivation, implementation	3	Lecture
Calculating Material Properties	3	Lecture
Hands-on #1 Lattice Constants and Bulk Moduli	3	Lecture & Experiment
Hands-on #2 Point Defects	3	Experiment
Modeling and simulation of material processes	3	Lecture
Hands-on #3 Dislocations	3	Lecture & Experiment
Hands-on #4 Hopping	3	Lecture & Experiment
Frontiers: Materials Genome and related tools	3	Lecture & Experiment
Density functional theory: introduction	3	Lecture
DFT calculations for crystals	3	Lecture
DFT calculations: practical concerns	3	Lecture
Hands-on #6 basic DFT calculation	3	Lecture & Experiment
Hands-on #7 lattice constants, and band structure calculations	3	Lecture & Experiment
Multiscale modeling: concepts, approaches, and applications	3	Lecture

*教学大纲（English）Syllabus	（须与中文一致，翻译请力求信达雅。） 教学内容 Content / 授课学时 Hours / 教学方式 Format Introduction: scientific computation and scientific programming — 3 — Lecture Molecular Dynamics methods: principles, algorithm, implementation, codes — 3 — Lecture Interatomic potentials: theory, derivation, implementation — 3 — Lecture Calculating Material Properties — 3 — Lecture Hands-on #1 Lattice Constants and Bulk Moduli — 3 — Lecture & Experiment Hands-on #2 Point Defects — 3 — Experiment Modeling and simulation of material processes — 3 — Lecture Hands-on #3 Dislocations — 3 — Lecture & Experiment Hands-on #4 Hopping — 3 — Lecture & Experiment Frontiers: Materials Genome and related tools — 3 — Lecture & Experiment Density functional theory: introduction — 3 — Lecture DFT calculations for crystals — 3 — Lecture DFT calculations: practical concerns — 3 — Lecture Hands-on #6 basic DFT calculation — 3 — Lecture & Experiment Hands-on #7 lattice constants, and band structure calculations — 3 — Lecture & Experiment Multiscale modeling: concepts, approaches, and applications — 3 — Lecture
*课程要求（中文）Requirements	（课程考核方式、考核标准等；不少于 50 字） 课程考核采用综合评价的方式，包括以下几个方面：

	1）课程作业 30%； 2）随堂测试 20%； 3）实验报告 40%； 4）课堂参与 10%。 具体比例每学期会有所调整，以教学班公布为准。
*课程要求 （English） Requirements	（须与中文一致，翻译请力求信达雅。） The grading of this course will be based on the comprehensive assessing of the following items: 1) Course assignments 30%; 2) In class quizzes 20%; 3) Experimental reports 40%; 4) Class attendance and participation 10%. The ratios of each parts might subject to change for different semester.
*课程资源 （中文） Resources	（教材、教参、网站资料等。） 参考资料： 1. June Gunn Lee, *Computational Materials Science: An Introduction,* CRC press, 2016. 2. Richard LeSar, *Introduction to Computational Materials Science Fundamentals to Applications*, Cambridge University Press, 2013. 3. D. Frenkel and B. Smit. Understanding Molecular Simulation. 2nd ed. Burlington, MA: Academic Press, 2001. 4. K Capelle, A Bird’ s-Eye View of Density-Functional Theory, Brazilian Journal of Physics, 36(4A):1318-1343, 2006. 5. Ellad B. Tadmor and Ronald E. Miller, Modeling Materials: Continuum, Atomistic and Multiscale Techniques, Cambridge University Press, 2011. 6. S. Yip, Handbook of Materials Modeling, Springer, New York, 2005.
*课程资源 （English） Resources	（须与中文一致，请力求信达雅。） References: 1. June Gunn Lee, *Computational Materials Science: An Introduction,* CRC press, 2016. 2. Richard LeSar, *Introduction to Computational Materials Science Fundamentals to Applications*, Cambridge University Press, 2013. 3. D. Frenkel and B. Smit. Understanding Molecular Simulation. 2nd ed. Burlington, MA: Academic Press, 2001. 4. K Capelle, A Bird’ s-Eye View of Density-Functional Theory, Brazilian Journal of Physics, 36(4A):1318-1343, 2006. 5. Ellad B. Tadmor and Ronald E. Miller, Modeling Materials: Continuum, Atomistic and Multiscale Techniques, Cambridge University Press, 2011. 6. S. Yip, Handbook of Materials Modeling, Springer, New York, 2005.
备注 Note	