* Semester	Fall	* Cross-semester?	No	Spanning over Semesters
* Course Type	Program Core Course	* Course Type	For full-time students	
* Course Category	Specialized Course	Targeting Students	All graduates	
* Instruction Language	English	Teaching Method	In class teaching	
* Grade	Letter grading	Exam Method	Hand-on	
* School				
Subject				

Person in charge	Name	ID	School	E-mail
				konglt@sjtu.edu.cn

Extended Information	
* ( ) Course Description	200 “ - ”
* English Course Description	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.

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Syllabus

Content	Hours	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

* English Syllabus	

Content	Hours	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

* Requirements	50

	1) 30% 2) 20% 3) 40% 4) 10%
* English Requirements	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.
* Resources	
* English Resources	References:
Note	