<table>
<tr><td></td><td colspan="2"></td><td></td><td colspan="3"></td></tr>
<tr><td>* Semester</td><td colspan="2">Fall</td><td>* Cross-semester?</td><td>No</td><td colspan="2">Spanning over Semesters</td></tr>
<tr><td>* Course Type</td><td colspan="2">Program Core Course</td><td>* Course Type</td><td colspan="3">For full-time students</td></tr>
<tr><td>* Course Category</td><td colspan="2">Specialized Course</td><td>Targeting Students</td><td colspan="3">All graduates</td></tr>
<tr><td>* Instruction Language</td><td colspan="2">English</td><td>Teaching Method</td><td colspan="3">In class teaching</td></tr>
<tr><td>* Grade</td><td colspan="2">Letter grading</td><td>Exam Method</td><td colspan="3">Hand-on</td></tr>
<tr><td>* School</td><td colspan="6"></td></tr>
<tr><td>Subject</td><td colspan="6"></td></tr>
<tr><td rowspan="2">Person in charge</td><td>Name</td><td>ID</td><td colspan="2">School</td><td colspan="2">E-mail</td></tr>
<tr><td></td><td></td><td colspan="2"></td><td colspan="2">konglt@sjtu.edu.cn</td></tr>
<tr><th colspan="7">Extended Information</th></tr>
<tr><td>* ( ) Course Description</td><td colspan="6">200
-</td></tr>
<tr><td>* English Course Description</td><td colspan="6">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>
</table>

*
( )
Syllabus

Modeling and simulation of material processes		
Hands-on #3 Dislocations		
DFT calculations: practical concerns		

* English Syllabus	<table><tr><td></td><td></td><td></td></tr><tr><td></td><td></td><td></td></tr><tr><td></td><td></td><td></td></tr><tr><td></td><td></td><td></td></tr><tr><td></td><td></td><td></td></tr><tr><td></td><td></td><td></td></tr><tr><td></td><td></td><td></td></tr><tr><td>Modeling and simulation of material processes</td><td></td><td></td></tr><tr><td>Hands-on #3 Dislocations</td><td></td><td></td></tr><tr><td></td><td></td><td></td></tr><tr><td></td><td></td><td></td></tr><tr><td></td><td></td><td></td></tr><tr><td></td><td></td><td></td></tr><tr><td>DFT calculations: practical concerns</td><td></td><td></td></tr><tr><td></td><td></td><td></td></tr><tr><td></td><td></td><td></td></tr><tr><td></td><td></td><td></td></tr></table>
* Requirements	50

* 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	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.
* English Resources	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.
Note	