Technical Elective: Computational Materials Science

Instructor
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Meeting Time & Location
Lecture & Lab: Monday 13:50-16:25 at RM 4-212

Office Hours
Wednesday-Friday: 13:00-16:00

TA Information
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Course Catalog Description
Theories of materials science from first principles to constitutive laws. Materials modeling and computer simulation at multiple length and time scales. Laboratory practice of various computational methods. Hands-on experience in code development and programming.

Course Materials
Lecture notes and handouts; No textbook.

Copyrights
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Prerequisites
Basic programming skill in at least one of the following environments: Mathematica, Matlab, Fortran, C, C++, Python …

Course Objectives
Upon successful completion of this course, a student will be able to
1. apply some fundamental theories of materials science from first principles to continuum constitutive laws;

2. model and simulate basic material structure and property at multiple length and time scales;
3. select appropriate computational tools for specific problems based on the advantages and limitations of different computational methods;
4. perform computational materials research by using available software;
5. develop custom code of selected materials topics in one computing environment.

Topics Covered
1. Quantum Mechanics and Density Functional Theory
2. Molecular Dynamics
3. Statistical Thermodynamics & Monte Carlo method
4. Binary Solid Solution
5. Phase Field Modeling
6. Finite Element Method

Grading
30%: participation in class lectures and lab instructions
40%: lab reports (weekly mini-projects as homework/lab practice)
30%: term project report and oral presentation

Late Assignment Policy
10% deduction/day

Grade Policy

A: 90 – 100	A−: 85 – 90	B+: 80 – 84	B: 76 – 80	B−: 73 – 76
C+: 70 – 73	C: 66 – 70	C−: 63 – 66	D: 60 – 63	F: < 60

Academic Integrity
All students are expected to adhere to the standards of academic honesty. Any student engaged in cheating, plagiarism, or other acts of academic dishonesty would be subject to disciplinary action. Any student suspected of violating this obligation for any reason during the semester will be required to participate in the procedural process, initiated at the instructor level, as outlined in the University Guidelines on Academic Integrity. This may include but is not limited to the confiscation of the examination of any individual suspected of violating the University Policy.

Term Project

<u>Requirement:</u> Written Report + Oral Presentation

<u>Idea:</u>

1. Use what you learn in this course to find a topic/problem and solve it. (must be your own idea, never cheat or plagiarize)
2. Try to learn a new software we don't show in class and use apply it to a specific problem. (DFT: VASP, ABINIT …; Molecular dynamics: feram, AMBER, OPLS …; Monte Carlo: BOSS, MacroModel …)
3. Try to reprogram the Spinodal Decomposition code by using a different language. (C, C++, Matlab …)
4. Build your own mathematical model and develop a program by yourself to solve the problem in materials science.

<u>Written Report Format:</u>

1. Introduction
Brief description of the background of your project research topic, with a few relevant references. You are expected to understand the general concepts of the topic and identify at least one problem to solve (not necessarily unsolved in literature), into which you propose to gain some insight by using computer modeling and simulation.

2. Methodology
Mathematical formulation of the model of your research problem (if relevant), numerical method used to solve the equations (if relevant), and input parameters used in your simulations (if relevant).

3. Results and Discussion
Simulation results to shed some light on the problem(s) of your interest. Discussion is What you want to say about your research project (limited to/based on your results).

4. Conclusion
Briefly summarize your main findings.

5. References
Key references.

<u>Oral Presentation:</u>
5-10 minutes' seminar-style computer-based presentation, followed by a question-and-answer part in class.