CBE/MECH 680
Advanced Computational Methods for Materials

COURSE OUTLINE

Spring 2008
T&R 11:00-12:15
107B Wagar

TEXTBOOK:	No required textbook. Lecture notes and handouts will be used.
REFERENCE BOOKS:	Levine, ***Quantum Chemistry***, 2nd Ed., Allyn and Bacon, 1974; Dronskowski, ***Computational Chemistry of Solid State Materials***, Wiley-VCH, 2005; Ashcroft/Mermin, ***Solid State Physics***, Holt, Rinehart and Winston, 1974; Leszczynski (edit), ***Computational Materials Science***, Elsevier, 2004; Thijssen, ***Computational Physics***, Cambridge University Press, 1999; Allen & Tildesley, ***Computer Simulation of Liquids***, Oxford, 1987; Frenkel & Smit, ***Understanding Molecular Simulation: From Algorithms to Applications***, 2nd Ed., Academic, 2002.
INSTRUCTORS & OFFICE HOURS:	Dr. **Xianghong Qian**, Dept. of Mechanical Engineering (Tuesday, 2~3 pm. Office: AR103 Engineering, Phone: 491-0992. Email: xhqian@engr.colostate.edu) Dr. **Qiang (David) Wang**, Dept. of Chemical and Biological Engineering (Tuesday, 4~5pm. Office: 108 Glover. Phone: 491-2763. E-mail: q.wang@colostate.edu)
HOMEWORK:	There will be several homework assignments. Students may help each other, but copying is not allowed. Assignments are due at the beginning of class. Each assignment must be submitted on the indicated due date and will be graded. Late homework may (and should!) be turned in, but 20% will be deducted for each day that it is late. ***Homework done using homework solutions from any source will receive 0 credit***. **Homework results represent 30% of the grade for the course**.
PROJECT:	Each student will be assigned a semester project to be completed independently. A written report and an oral presentation are required for the project; the report will be graded by the instructors, and the presentation will be graded by the audience (including rest of the class and instructors). **The project results represent 30% of the grade for the course**.
EXAMINATION:	There will be only one final exam for this course, which is close-book but 1-page (letter-size) notes and a calculator can be used. **The final exam results represent 40% of the grade for the course**.
COMMENTS:	The primary objective of this highly interdisciplinary course is to provide an overview of the commonly used advanced computational methods in cutting-edge research in Materials. The emphasis is on the basic principles and applicability of these methods, as well as their interconnections. Students will have hands-on computer simulation experience without programming. **Thermodynamics, Calculus, Physical Chemistry or equivalent at the undergraduate level are needed for taking this course.**

Additional Information

Academic Integrity Policy

A statement of the university's academic integrity policy can be found in the General Catalog at http://www.catalog.colostate.edu/front/policies.aspx (scroll down to the section on "Students' Responsibilities"). The policy is zero tolerance. The ***minimum*** action taken for academic dishonesty will be a failing grade for the course. In particular:

- Students may not copy any part of a homework assignment or an exam from other students, ***including from previous years***. The student who knowingly provides his/her assignment or exam to be copied is also in violation of the CSU policy. Students, however, are allowed and encouraged to work in groups on homework assignments.
- Students are forbidden to use solution manuals from any source. The resources that the students are allowed to use for homework and exams are limited to textbook, reference or similar books, lecture notes and handouts, and data handbooks. For the project, other resources may be used.
- Discussing the content of an exam with someone who has not taken the exam is not allowed.

Semester project

Some examples of the topics for the project are: determining the lattice constants of a bulk crystalline material, calculating NMR spectroscopy, finding an optimal structure of a polysaccharide molecule, summarizing the recent advances in a computational method, etc. Each student should discuss with the instructor about his/her selected topic and scope. The presentation should be well organized (no longer than 15 minutes, including questions). Blackboard and computer projector are available for the presentation. All presentations will be given in the last week of class, and will be graded by the audience on a scale of 1~10 (1 for the worst and 10 for the best presentation you've ever had).

Learning objectives

The student successfully completing this course will be able to:

1. Learn the basic methodology in computer simulations in materials science and engineering;
2. Describe the basic principles of various computational methods, their applicable time and length scales, and their interconnections;
3. Choose appropriate computational methods to solve targeted problems;
4. Apply quantum mechanical methods and use various software packages;
5. Explain how molecular simulations (molecular dynamics and Monte Carlo simulations) work;
6. Derive the acceptance criteria for Monte Carlo trial moves in various ensembles;
7. Calculate entropy-related quantities (chemical potential, free energies) in molecular simulations using various methods;
8. Apply variational calculus to derive the governing equations in density-functional theory and mesoscopic simulations.

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Preliminary Class Schedule (1-17-08)

Week	Topic(s)
1 (Jan. 22 & 24)	Introduction to Scientific Computing
2 (Jan. 29 & 31)	Fundamentals of Variational Calculus
3 (Feb. 5 & 7)	Fundamentals of Quantum Chemistry
4 (Feb. 12 & 14)	Ab initio Calculations
5 (Feb. 19 & 21)	Density Functional Theory
6 (Feb. 26 & 28)	Tight-Binding and Semi-empirical Calculations
7 (Mar. 4 & 6)	Fundamentals of Statistical Mechanics
8 (Mar. 11 & 13)	Ab initio Molecular Dynamics Simulations
9 (Mar. 18 & 20)	***No Class (Spring Recess)***
10 (Mar. 25 & 27)	Classical Molecular Dynamics Simulations
11 (Apr. 1 & 3)	Basic Monte Carlo Simulations
12 (Apr. 8 & 10)	Advanced Monte Carlo Simulations
13 (Apr. 15 & 17)	Phase-Field Modeling
14 (Apr. 22 & 24)	Phenomenological Models using Functional Minimization
15 (Apr. 29 & May 1)	Introduction to Supercomputing and Multi-scale Modeling
16 (May 6 & 8)	Project Presentations
1:30~3:30pm, May 15	***Final Exam***

Note: this schedule may change as the course progresses.