EMA 6804 – Quantum Methods in Computational Materials Science

Course Syllabus – Spring 2016

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Course Description (3 credit hours)

Theory, methods, and application of common quantum mechanical software for computational study of materials.

Prerequisites:

EMA 6316 - Materials Thermodynamics
Python, Java, C/C++, Fortran, or any other suitable scientific programming language.

Course Objectives

This is a graduate level course. It introduces state-of-the-art computational methods for materials research with emphasis on the atomic and nano scales and hands-on modeling on PCs and supercomputers. The class is aimed at beginning graduate students and will introduce a variety of computational methods used in different fields of materials science. The main focus is quantum mechanical methods with a short overview of atomistic methods for modeling materials. These methods will be applied to the properties of real materials, such as electronic structure, mechanical behavior, diffusion and phase transformations. The course will enable students to implement and employ a variety of current modeling methods relevant to a wide range of materials, from metals and semiconductors to ceramics and polymers to molecules and liquids.

Class Time

Tuesday	Period 3	9:35-10:25	CSE E122
Thursday	Period 3-4	9:35 - 11:30	CSE E122

Text books: (none required)

- D. J. Barrett, *Linux Pocket Guide* (O'Reilly, 2004).
- D. Sholl, *Density Functional Theory: A Practical Introduction* (Wiley, 2009).
- R. Martin, *Electronic structure: Basic theory and practical methods* (Cambridge, 2004).
- E. Kaxiras, *Atomic and Electronic Structure of Solids* (Cambridge, 2003).
- J. G. Lee, *Computational Materials Science: An Introduction* (CRC Press, 2011).
- F. Jensen, *Introduction to Computational Chemistry* (Wiley, 2006).

The reference texts are not explicitly used in the course. They provide additional material and explanations for the course topics. If you have difficulties with topics, it is up to you to seek out these references.

Course Website

The course website is on the Canvas system http://lss.at.ufl.edu, where you can find the syllabus, lecture notes, homework problems, announcements, and your grades. Please check it frequently.

Lectures

Lectures are critical to success in this MS&E course. However, I will not require attendance. Questions are highly encouraged. It will make the class more interesting, wake up your fellow students and give me a chance to explain things better. If you do not understand something, chances are that most of the class missed that point too. If you as students do not ask enough questions, I will start asking you.

Computer Lab

Most Tuesdays we will work on projects, discuss problems, and have special demonstrations and student presentations. You are expected to actively participate in these sessions, work in groups, discussing advanced topics or working on specific problems.

Homework, due Wednesdays at midnight

In the first part of the class, I will distribute four homework problems on a biweekly basis. Discussion of the homework may occur during the Tuesday sessions. The problems will cover the previous couple of lectures. Full detailed solutions will be provided for all problems.

Project

A significant part of the class will be devoted to a modeling project. Each student or team of two students will choose a modeling project. This could be a project related to your research interests or from a list of projects I will provide. The project will require independent work alone or in groups of two and students will either develop a computer program to model materials or use existing software to calculate materials properties. Students will submit a written project report and give a 20 minute presentation about their results as part of the lecture.

Grading

Grades will be based on your understanding and mastery of the material as demonstrated by quantitative scores on homework (67%) and the project report and presentation (33%).

Grading Scale

Percentage	≥92	≥88	≥84	≥80	≥76	≥72	≥68	≥65	≥62	≥59	≥56	<56
Letter Grade	A	A-	B+	B	B-	C+	C	C-	D+	D	D-	E
Grade Points	4.0	3.67	3.33	3.0	2.67	2.33	2.0	1.67	1.33	1.0	0.67	0

Office Hours

If I am in my office with the door open, you are welcome to come in and ask questions. A closed door means I am either not there or on a conference call, or writing an exam/proposal. Official office hours are Tuesday afternoons 3:00-4:00pm. I will try to respond to e-mail questions as fast as possible. Important e-mail questions (minus identifying information) and answers will be posted to the class either by e-mail or on the course website for the benefit of other students.

Honesty Policy

All students admitted to the University of Florida have signed a statement of academic honesty committing themselves to be honest in all academic work and understanding that failure to comply with this commitment will result in disciplinary action. This statement is a reminder to uphold your obligation as a UF student and to be honest in all work submitted and exams taken in this course and all others.

Note that failure to comply with this commitment will result in disciplinary action compliant with the UF Student Honor Code Procedures.
See http://www.dso.ufl.edu/sccr/procedures/honorcode.php.

Accommodation for Students with Disabilities

Students Requesting classroom accommodation must first register with the Dean of Students Office. That office will provide the student with documentation that he/she must provide to the course instructor when requesting accommodation.

UF Counseling Services

Resources are available on-campus for students having personal problems or lacking clear career and academic goals. The resources include:

- UF Counseling & Wellness Center, 3190 Radio Rd, 392-1575, psychological and psychiatric services.
- Career Resource Center, Reitz Union, 392-1601, career and job search services.

Software Use

All faculty, staff and student of the University are required and expected to obey the laws and legal agreements governing software use. Failure to do so can lead to monetary damages and/or criminal penalties for the individual violator. Because such violations are also against University policies and rules, disciplinary action will be taken as appropriate. We, the members of the University of Florida community, pledge to uphold ourselves and our peers to the highest standards of honesty and integrity.

Week	Class dates	Topics
1	January 5 January 7	What is Computational Materials? Introduction and examples.
2	January 12 January 14	Lab: Introduction to the computer environment. Basics of unix, parallel computers and batch systems. Lecture: Empirical energy models and force fields. Practical considerations for crystalline and molecular structures.
3	January 19 January 21	Lab: Crystal structure relaxation, defect energies, and elastic properties using empirical force fields. Lecture: Empirical many-body potentials for metals, semiconductors, ionic and bio-molecular materials.
4	January 26 January 28	Lab: Setting up molecular structures with Avogadro. Simulations of water and organic molecules. Lecture: Introduction to quantum mechanics of materials.
5	February 2 February 4	Lab: Quantum mechanical calculations of the molecular structure and HOMO-LUMO gaps of water using Gaussian. Importance of basis set convergence. Lecture: The Hartree and Hartree-Fock methods.
6	February 9 February 11	Lab: Quantum mechanical calculations of the molecular and electronic structure of acenes using Gaussian. Role of correlations. Lecture: Multi-determinant methods.
7	February 16 February 18	No class - Project work No class - Project work
8	February 23 February 25	Lab: Lecture: Density-functional theory.
9	March 1 March 3	Spring Break
10	March 8 March 10	Lab: Density functional calculations for energies and lattice parameters of silicon using the PWSCF code. Lecture: Practical aspects of density-functional theory, pseudopotentials, Brillouin zone integration, basis sets, etc.)
11	March 15 March 17	Lab: Calculation of the electronic bandstructure and bonding characteristic of III-V semiconductors using semi-local exchange-correlation functionals. Lecture: Successes and failures of density functional theory.
12	March 22 March 24	Lab: Calculation of electronic properties using hybrid exchange-correlation functionals. Lecture: Hybrid functionals and the GW method.
13	March 29 March 31	Lab: Calculation of the phonon spectra using Phonopy. Lecture: Density-functional perturbation theory.
14	April 5 April 7	Lab: Nudged-elastic band calculation for vacancy diffusion. Lecture: Transition state theory and infrequent event methods.
15	April 12 April 14	Project Reports Project Reports
16	April 19	Project Reports