Computational Nanoscience for Energy

Fall 2009 : 3.29 : TR 9:30-11 : Prof. Jeffrey Grossman : jcg@mit.edu
12 Units (3-0-9) : Graduate Course : Seniors with Permission

First Day Handout

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Format: This course will consist of two 1.5-hour lectures per week and hands-on, interactive simulation using research and commercial codes as well as web-based simulation codes such as those found at nanohub.org.

Prerequisites: Graduate standing or instructor approval.

Course Description: Materials for energy conversion and storage can be greatly improved by taking advantage of unique effects that occur at the nanoscale. In many cases, these improvements are due to fundamental microscopic mechanisms that can be understood and predicted by cutting-edge simulation methods. This course will provide students with the fundamentals of computational problem-solving techniques that are used to elucidate the atomic-scale behavior of energy conversion and storage nano-materials. Emphasis will be placed on how to use simulations effectively, intelligently, and cohesively to predict properties that occur at the nanoscale for problems in energy. Detailed examples of how computation can play a key role will be discussed for materials in thermoelectrics, solar fuels, solar photovoltaics, and hydrogen storage.

The course is designed to present a broad overview of computational nanoscience for energy and is suitable for both experimental and theoretical researchers. While some aspects of the simulation methods such as numerical algorithms will be presented, there will be little if any programming required. Rather, we will emphasize the intelligent application (as opposed to "black box" use) of codes and methods, and the connection between the computer results and the physical properties of the problem.

Class time will be spent predominantly on lectures and discussion, to some extent on in-class simulation, and at the end of the semester on student presentations. Homework assignments will be assigned roughly every two weeks, most of which involve the use of on-line simulation tools developed for this class on the nanoHUB. Students are encouraged to explore www.nanohub.org, create a user account, and become familiarized with the nanoHUB project.

Required Textbooks: Due to the wide-ranging nature of material covered in this class, there will be no specific required textbooks. A combination of published review articles and relevant books will be encouraged as reading material. In addition, Powerpoint presentations will be posted on the course web site and on the nanoHUB.

Homework: Homework will consist primarily of numerical experiments with existing codes, and a class project. We will stress the different computational approaches that are available for solving realistic problems related to nanomaterials for energy conversion and storage.

Grading: There are no exams. The breakdown of a final grade for this course is as follows:

<u>20% class participation:</u> your active participation during class is important, and simply showing up is mandatory.

<u>40% homework:</u> homework will consist mostly of numerical experiments with existing codes and at times of derivations related to the lectures. An in-class pop-quiz counts as one homework assignment. Working together on homework assignments is fine.

<u>40% class project:</u> class projects will consist of a written report based on simulations you carry out to solve a scientific problem of interest related to energy conversion or storage. This can be something directly related to your own research, or something that allows you to explore a certain realm of computational nanoscience for energy in more detail. It is required that you submit a 1-page (maximum) description of your project <u>no later than November 10</u>.

Class Etiquette: A few important items regarding etiquette:

Be on time. We will begin class at 9:30 AM.

Come to class prepared, and expect to be called on periodically.

Beverages are permitted in class, but food is not.

If you cannot make a class meeting, or if you will be late for class, send an e-mail to me advising of this in advance.

Laptops, PDAs, cell phones and similar electronic devices will be turned off during class and left in your backpack or briefcase. The only exception to this is for in-class simulation days.

Course Website: Please check the website for the syllabus and any changes to it, pdfs of the class lectures, homework assignments, a general discussion forum for the class, and possibly other useful information.

Tentative Schedule of Class Lectures:

9/10 Introduction: Organization of Class, Historical Perspective, "Computer Experiments," overview of energy conversion and storage materials and impact of nanotechnology

9/15 Energy conversion: thermoelectric materials

9/17 Thermoelectrics: impact of nanotechnology

9/22 Introduction to molecular dynamics and classical force fields

9/24 Basic classical MD simulations and analyses: energy minimization, geometry optimization, and seeing what you're doing

9/29 A day of class simulation: learning how to do MD simulations
→ Homework #1 assigned

10/1 Computing lattice thermal conductivity from classical MD to predict impact of nanostructuring

10/6 Energy storage: solar fuels
→ Homework #2 assigned

10/8 Solar fuels: impact of nanotechnology

10/13 Introduction to computational quantum mechanics beginning with quantum chemistry methods, molecular orbital calculations, tight-binding

10/15 Beyond Hartree-Fock and towards "chemical accuracy", plus reactions

10/20 A day of class simulation: tight-binding and Hartree-Fock Calculations
→ Homework #3 assigned

10/22 Computing reaction pathway energetics for a molecular solar fuel and "designing" a higher energy storage capacity

10/27 Energy conversion: solar photovoltaics
→ Homework #4 assigned

10/29 PV: impact of nanotechnology

11/3 Basic introduction to density functional theory

11/5 Electronic structure analyses: density of states, band structures, etc.

11/10 Density functional theory: what it does and doesn't do and in-class simulation
→ Homework #5 assigned

11/17 Computing charge separation properties in excitonic solar cells: ground and excited state densities and level alignments

11/24 Energy storage: hydrogen storage materials
→ Homework #6 assigned

11/26 Thanksgiving break

12/1 Hydrogen storage: the impact of nanotechnology

12/3 Introduction to near-exact methods: quantum Monte Carlo

12/7 In-class simulation day: QMC calculations for computing the tunability of hydrogen desorption in nanoparticles

12/10 class project presentations

12/10 class project presentations

12/15 class project presentations