16:155:520:01 Multiscale Materials Modeling Spring 2020

Web page: https://sakai.rutgers.edu
Lectures: Will be provided on course website before class.
Classroom: Engineering Building C115
Lecture Time: Wednesday, 5pm to 8pm
Instructor: Meenakshi Dutt
Engineering Building, Rm C-229
Busch Campus
Email: meenakshi.dutt@rutgers.edu
Office Hours: By appointment only.

Course Objectives:
To learn the fundamental concepts underlying computational models and methods to simulate and design hard and soft materials across spatiotemporal scales.

Course Description:
The course will cover computational models and methods for simulating the structural and dynamical characteristics of hard and soft materials at different spatiotemporal scales. Topics will include accurate first principles quantum-based methods, atomistic, molecular modeling, multi-scale approaches and continuum techniques. Emerging computational methods related to diverse aspects of materials modeling will also be covered. The discussion of the various topics will be accompanied by case studies from research papers.

Course Software:
Software from various external sites will be used for the assignments. Instructions will be provided in the relevant assignments. MATLAB/MAPLE may be required for plotting graphs and data analysis.

Pre-requisites:
Introductory Physics and Chemistry; Advanced Engineering Mathematics; Introductory Statistical Mechanics, Thermodynamics and Transport. Basic understanding of hard and soft materials. Proficiency with a computing language (for example, C/C++/MATLAB). The course is designed for students in first or second year of engineering and science graduate programs and motivated seniors with interest in modeling of materials at different scales.

Computing Requirements:
Rutgers NET ID is required to access course material on course website.

Textbook:
Numerous textbooks will be used through the lecture series. The instructor will provide the relevant book chapters associated with each lecture. All course material will be available on the class sakai resources.

Class Participation:

Class participation and attendance is essential.

Assessment:
Home works (5) and Literature Review: 60%, Project: 40%. The project is group-based and has a class presentation. All assignments are compulsory and must be submitted by the deadline.

Home works and Literature Review:
Reading assignments in the form of research papers, reviews and book chapters will be assigned every week and discussed during class. Each reading assignment will be accompanied by hands-on computer work, and will include a series of questions to be turned in and graded.

Projects:
One hands-on computational project will be required in lieu of a midterm and final exam.

Course Timetable:

Lecture	Date	Topic
1	01/22	Overview to materials; relevant spatiotemporal scales; types of materials; modeling of materials; course overview; review of nanotechnology.
2	01/29	Review of quantum theory; introduction to the wave equation and wave function
3	02/05	Computational tools of quantum mechanics: Hartree-Fock, Basis Sets; Density Functional Theory and Semi-Empirical Methods
4	02/12	
5	02/19	Molecular Mechanics, Classical Mechanics, Statistical Mechanics, Molecular Dynamics and Monte Carlo Methods
6	02/26	
7	03/04	
8	03/11	
9	03/25**	Analysis of Simulation Outputs, Potentials for Hard and Soft Materials
10	04/01	Coarse-grained molecular simulations
11	04/08	Mesoscopic simulation methods: Event Driven Molecular Dynamics, Dissipative Particle Dynamics, Finite Element Modeling
12	04/15**	
13	04/22	Special Topics on Emerging Computational Methods for Designing Materials; Class Summary and discussions
14	04/29	Project presentations

Note: No classes on March 18, 2020 (Spring break). ** Classes on March 25, 2020 and April 15, 2020 may be rescheduled due to instructor travel. Make-up classes will be held in C115 on dates to be scheduled after discussion with class.

Academic Integrity
Students are expected to familiarize themselves with and adhere to the University policy on academic integrity at:

http://academicintegrity.rutgers.edu/files/documents/AI_Policy_2013.pdf

and the Code of Student Conduct at

http://studentconduct.rutgers.edu/files/documents/UCSC_2013.pdf.

It is understood that a student's name on any individual homework assignment, quiz, or exam indicates that he/she neither gave nor received unauthorized aid. On individual homework assignments, authorized aid includes discussing: 1) interpretation of the problem statement, 2) concepts involved in the problem, 3) approaches for solving the problem. Anything beyond this constitutes unauthorized aid and violates the academic integrity policy. A student's name on a group assignment indicates that he/she contributed to the assignment. Disciplinary actions for academic misconduct will be in accord with the University policy on academic integrity. At a minimum, a first offense will result in a zero for the assignment. The penalty for repeat offenses will be significantly more severe. A second offense will result in a failing grade for the course.

The principles of academic integrity require that a Rutgers student:

- properly acknowledge and cite all use of the ideas, results, or words of others.
- properly acknowledge all contributors to a given piece of work.
- make sure that all work submitted as his or her own in a course or other academic activity is produced without the aid of impermissible materials or impermissible collaboration.
- obtain all data or results by ethical means and report them accurately without suppressing any results inconsistent with his or her interpretation or conclusions.
- treat all other students in an ethical manner, respecting their integrity and right to pursue their educational goals without interference. This requires that a student neither facilitate academic dishonesty by others nor obstruct their academic progress.
- uphold the canons of the ethical or professional code of the profession for which he or she is preparing.