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SCHOOL OF MATERIALS ENGINEERING

To:	**Engineering Curriculum Committee**	**EFD# 2-19**
From:	**David F. Bahr, Head School of Materials Engineering**	
Date:	**March 4, 2019**	
Subject:	**Proposal for New Graduate Course**	

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Course Number:	MSE 67000
Course Title:	Atomistic view of materials: theory, modeling and simulations
Short Title:	Atom View Matls: T M & S

Previously taught as:	MSE 69700: F14, F15, F16, F17, F18
Course:	3 credit hour, lecture
Proposed offering:	Spring, fall or summer

Course Description:

In "Atomistic View of Materials: Theory, Modeling & Simulation" students will be introduced to the fundamental physics required to describe materials in terms of electrons and atoms, learn how these processes relate to macroscopic behavior and become familiar with advanced modeling and simulation techniques that enable quantitative predictions. Students will gain hands-on experience with several simulation tools, including ab initio calculations using density functional theory, molecular dynamics simulations and other advanced modeling techniques.

Course Syllabus

A. MSE 67000 - Atomistic View of Materials: Modeling & Simulation

B. Instructor

Prof. Alejandro Strachan

C. Course description

In "Atomistic View of Materials: Theory, Modeling & Simulation" students will be introduced to the fundamental physics required to describe materials in terms of electrons and atoms, learn how these processes relate to macroscopic behavior and become familiar with advanced modeling and simulation techniques that enable quantitative predictions.

Students will perform hands-on, ab initio calculations using density functional theory and other advanced techniques as well as molecular dynamics simulations.

D. Topics

- The quantum mechanics of bonding and electronic structure
  - Atoms, molecules and crystals
- Electronic structure calculations
  - Hartree-Fock & post-Hartree-Fock methods
  - Density functional theory
  - Beyond density functional theory
  - Response function predictions and electronic structure for molecules, crystals and hybrid materials
- Classical and statistical mechanics
  - Hamilton's formalism of classical mechanics
  - Normal modes and phonons
  - Statistical mechanics (classical, Bose-Einstein, and Fermi-Dirac)
  - Kinetic theory and Boltzmann transport equation
- Molecular dynamics simulations
  - Interatomic potentials for various classes of materials (e.g. embedded atom model, ReaxFF)
  - Computing the thermo-mechanical response of materials
- Dynamics with Implicit Degrees of Freedom
  - Coarse grained simulations of molecular materials
  - Two temperature model and electronic thermal transport
  - Atomistic simulations of electrochemical reactions

E. Learning objectives

By the end of the course, students are expected to be able to i) design, perform and analyze computer experiments using electronic and atomistic simulation techniques appropriate for the problem at hand, ii) be able to extract materials properties from the simulations; iii) recognize the approximations and estimate the level of accuracy to be expected from each modeling technique, and iv) be able to critically read the current scientific literature on computational modeling and simulation of materials.

F. Course organization

This course combines an online component with in-person lectures and hands-on activities. The online component will be through edX:

https://www.edx.org/course/atoms-materials-predictive-theory-purduex-mse550x

Students should register, for free, to the online class. This course will include advanced topics not contained in the online course and those will be covered though in-person lectures. In-person lectures will also be used to discuss hand-on simulations.

Homework assignments will also include online and in-person components and are designed for students to work on the topics discussed in class and gain first-hand experience with the simulations. These assignments will be graded as either complete or incomplete; in order to receive a passing grade students should not have more than one incomplete homework assignment.

An open-ended special project will be assigned during the first half of the semester and students will utilize the knowledge gained in the class to tackle the problem. Quizzes will be given in class to evaluate student progress. The final exam will be take-home, and comprehensive; it will be designed to evaluate whether the students achieved the learning objectives of the course.

G. Grading Policy

Project Report	40%
Quizzes	20%
Final Exam (take home)	40%

H. Prerequisites

Students will be expected to have working knowledge of college-level physics and math. Significant background materials will be provided during the course to accommodate students with diverse backgrounds. Minimal programing knowledge will be required to work on simple simulation codes and understand their inner workings. Background information and tutorials on this topic will also be provided.