**Department of Materials Science and Engineering**
**University of Maryland, College Park, Maryland**

1. **ENMA 400 – Introduction to Atomistic Modeling in Materials Science**

2. **Credits and contact hours – 3 credits.** The University of Maryland follows the Maryland Higher Education Commission's policies on "contact hours;" specifically, one semester hour of credit will be awarded for a minimum of 15 hours, of 50 minutes each of actual class time, exclusive of registration, study days, and holidays.

   **Schedule**: meets two 75 minute periods per week

3. **Instructor's or course coordinator's name: Prof. Yifei Mo**

4. **Text book, title, author and year:** no text book required
   a. **Other supplemental materials:** *Understanding molecular simulation: from algorithms to applications* / Daan, Frenkel, Berend Smit. (ebook available); **–** *Computer simulation of liquids* / M.P. Allen and D.J. Tildesley, *Molecular modelling: principles and applications* / Andrew R. Leach (at Chemistry Library reserves desk); *The ABC of DFT /* Kieron Burke and friends (ebook available); *Density functional theory: a practical introduction* / David S. Sholl, Janice A. Steckel (ebook available); *Introduction to modern statistical mechanics* / David Chandler; *Statistical mechanics* / Donald A. McQuarrie; *Introduction to solid state physics* / Charles Kittel; *Solid state physics* / Neil W. Ashcroft, N. David Mermin

5. **Specific course information**
   a. **Brief description of the content of the course (catalog description):** This is an introductory course aiming for junior and senior undergraduate students and graduate students to study atomistic modeling and simulation techniques. This course covers the theories, methods, and applications of atomistic-scale modeling techniques to simulate, understand, and predict the properties of materials. Specific Topics include: Molecular statics, Quantum mechanical methods; Molecular dynamics simulations and Monte Carlo simulations.

   b. **Pre-requisites or co-requisites:** ENMA 300; MATH 206; ENMA 460 and knowledge of Thermodynamics, Physical Chemistry or equivalent. Basic knowledge of quantum and statistical mechanics recommended.

   c. **Indicate whether a required, elective, or selected elective (as per Table 5-1) course in the program:** ENMA 400 is an elective course for Materials Science and Engineering majors.

6. **Specific goals for the course:**
   a. **Specific outcomes of instruction:** The main objective of this course is to:
      1. Student learns the key concepts of atomistic modeling and is able to perform computer modeling of materials.

   **b. Explicitly indicate which of the student outcomes listed in Criterion 3 or any other outcomes are addressed in this course**.
   ABET A: Ability to apply mathematics, science and engineering principles to design
   ABET C: Ability to design a system, component, or process to meet desired needs.
   ABET E: Ability to identify, formulate and solve engineering problems

7. **Brief list of topics to be covered:**

1. Introduction to atomistic modeling
2. Computers, Languages, and Introduction to MATLAB
3. Classical Mechanics
4. Molecular Statics
   Lab1: Unix & HPC. Get familiar with Deepthought
5. Classical potential I - Basic pair potentials
6. Classical potential II - Many-body potentials
   Lab 2: Molecular StaticsM
7. Molecular Dynamics I - Integrating F=ma, time steps;
8. Molecular Dynamics II - Thermostat
9. Molecular Dynamics III - Simulation analysis, limitations
   Lab 3: Molecular Dynamics
10. Quantum Mechanics I: Introduction
11. Quantum Methods II: Basic Applications Final project assigned
12. Quantum Methods III: Key Concepts of DFT
13. Quantum Methods IV: Introduction to VASP
    Lab 4: Quantum Mechanics - DFT1
14. Quantum Methods V: Applications and Materials Project
    Lab 5: Quantum Mechanics - DFT2
15. Monte Carlo I - State space sampling, Classical momentum
16. Monte Carlo II - Metropolis algorithm, simulation analysis
17. Advanced topics: Kinetic Monte Carlo; Accelerated MD.