

## CHEN E4880 – Syllabus – Spring 2020

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**Lectures:** Tue/Thu 1:10 pm – 2:25 pm, 214 Pupin Laboratories

**Office Hours:** Mon/Thu 2:30 pm – 3:30 pm, 812 Mudd

**Course Description:** This course is aimed at senior undergraduates and graduate students. The course covers atomistic simulation techniques for applications at the interface of chemical engineering and materials science. Students will learn the theoretical background of various simulation techniques ranging from empirical to first-principles approaches and will get hands-on experience in using state-of-the-art (free and open source) simulation software. Practical examples will focus on inorganic materials most of which will be crystalline solids, though the methods taught are transferable to other materials classes. Course grades are based on reports for practical assignments.

**Textbooks:** No specific textbook is required or recommended for this course. Primary literature, scientific reviews, and/or textbook chapters for each subject will be pointed out.

**Course Outcomes:**

- Working knowledge of the most common atomistic simulation techniques.
- Improved ability to understand/assess results from atomistic simulations.
- Basic knowledge of state-of-the-art simulation software.

**Modules and Projects:** The course consists of four modules: (1) Interatomic Potentials, (2) Density-Functional Theory, (3) Monte Carlo Simulations, and (4) Molecular Dynamics Simulations. In each module, the required technical background is first introduced, which is followed by a hands-on lab in which a project assignment is discussed. For each project, roughly three weeks will be available to complete the assignment.

**Course Grade:** 100% of the course grade will be based on the four projects/assignments. There is no exam. The report for each project will count 1/4 of the final grade.

**Collaborations:** All outcomes (written reports, input files, output files, scripts, etc.) must be the product of your efforts. However, you may discuss with anyone in the present class for help in solving the practical assignments. It is not permissible to speak to others (outside your classmates) about your projects. It is strongly encouraged that you work with classmates! However, if you collaborate with your peers, it must be documented. Failure to reference all who helped will be considered plagiarism. Discussions with others (including seniors) about the project, or looking at previous year solutions, if available, will be considered plagiarism.

**Policy for Late Submissions:** Reports are due at 11:59 pm on the due date. 10% will be deducted if late by less than 24 hours. 20% off for submissions that are late by 24-48 hours, and so on.

**Lecture Schedule and Due Dates (Subject to Changes):**

1. Tue, 01/21 Introduction and Overview
2. Thu, 01/23 Basic Crystallography
3. Tue, 01/28 Interatomic Potentials (Part I)
4. Thu, 01/30 Interatomic Potentials (Part II)
5. Tue, 02/04 Practical Considerations using Interatomic Potentials; Preparations for Lab 1
6. Thu, 02/06 **Lab 1: Interatomic Potentials**
7. Tue, 02/11 Basics of Quantum Mechanics
8. Thu, 02/13 Density-Functional Theory (DFT)
9. Tue, 02/18 Practical DFT Part I: Predicting Properties of Li-Ion Batteries
10. Thu, 02/20 Practical DFT Part II: Heterogeneous Catalysis
11. Tue, 02/25 Practical Considerations and Failures of DFT; Preparations for Lab 2; **Lab 1 Due**
12. Thu, 02/27 **Lab 2: DFT Calculations**
13. Tue, 03/03 [Guest Lecture: J. A. Garrido Torres – AI-Accelerated DFT Calculations](#)
14. Thu, 03/05 Basic Statistical Mechanics
15. Tue, 03/10 Fundamentals of Monte Carlo (MC) Simulations
16. Thu, 03/12 Advanced MC Topics
- 03/16-03/20 *Spring Recess*
17. Tue, 03/24 **Lab 3: MC Simulations; Lab 2 Due**
18. Thu, 03/26 Fundamentals of Molecular Dynamics (MD) Simulations
19. Tue, 03/31 Static Properties from MD: Equilibrium Structure
20. Thu, 04/02 Dynamic Properties from MD: Mass Transport (Diffusion)
21. Tue, 04/07 *Ab-Initio* MD Simulations
22. Thu, 04/09 Accelerated MD Simulations; **Lab 3 Due**
23. Tue, 04/14 **Lab 4: MD Simulations**
24. Thu, 04/16 [Guest Lecture: N. Artrith – Machine-Learning Models for MD Simulations](#)
25. Tue, 04/21 Computational Prediction of Atomic Structures
26. Thu, 04/23 Automated High-Throughput DFT Calculations
27. Tue, 04/28 Current Research and Future Directions in Atomistic Simulations
28. Thu, 04/30 Recap and Q&A; **Lab 4 Due**

### CHEN E4880 – Tentative Lecture Schedule (Subject to Changes)

Changes may arise and regular attendance in class is the best way to be informed.  
Changes in due dates will be posted in CourseWorks.

	Tue	Thu	Tue	Thu	Tue	Thu
1/21	1/23	1/28	1/30	2/4	2/6	2/6
Introduction and Overview	Basic Crystallography	Interatomic Potentials (Part I)	Interatomic Potentials (Part II)	Preparations for Lab 1	Lab 1: Interatomic Potentials	
2/11	2/13	2/18	2/20	2/25	2/27	2/27
Basic Quantum Mechanics	Density-Functional Theory (DFT)	DFT for Li-Ion Batteries	DFT for Heterogeneous Catalysis	Failures of DFT Preparations for Lab 2 Lab 1 Due	Lab 2: DFT Calculations	
3/3	3/5	3/10	3/12	3/17	3/19	3/19
Guest Lecture: AI-Accelerated DFT (J. A. Garrido Torres)	Basic Statistical Mechanics	Monte Carlo (MC) Simulations	Advanced MC Topics Preparations for Lab 3	Spring Recess		
3/24	3/26	3/31	4/2	4/7	4/9	4/9
Lab 3: MC Simulations Lab 2 Due	Molecular Dynamics (MD) Simulations	Static Properties from MD (Structure)	Dynamic Properties from MD (Transport)	Ab-Initio MD	Accelerated MD Lab 3 Due	
4/14	4/16	4/21	4/23	4/28	4/30	4/30
Lab 4: MD Simulations	Guest Lecture: ANN Models for MD (N. Artrith)	Atomic Structure Prediction	Automation	Current Research and Future Directions	Recap Q&A Lab 4 Due	