CHE 7120
Class # 15066
Molecular Simulations
Spring 2019 Syllabus
Ohio University
Department of chemical and Biomolecular Engineering

Instructor: Sumit Sharma, PhD
Office: 181 Stocker Center
Phone: 593-1425
E-mail: sharmas@ohio.edu

Class: 12 PM – 1.20 PM, T/Th, ARC 146
Office Hours: 9 – 10 AM, T/W/Th
Other times by appointment, requested 24 h in advance

Class e-mail: Make sure to check your email routinely as it will be used to communicate with you at times. E-mail will be considered an official way to communicate with the class. If you need to communicate via e-mail, you must use your official university account.

Required text: Computer Simulations of Liquids, M. P. Allen, D. J. Tildesley, Oxford Science Publications

Recommended texts:
1. Understanding Molecular Simulation: From Algorithms to Applications, D. Frenkel, B. Smit, Academic Press
2. Statistical Mechanics: Theory and Molecular Simulation, M. E. Tuckerman, Oxford Graduate Texts

Grading:

Molecular dynamics assignment:	25%
Monte Carlo assignment:	25%
Topic presentations:	25%
Homework assignments:	20%
Class participation:	5%

Class Etiquette: Use of cellphones are not allowed. No texting, web-browsing during the class. Your phones should be in silent mode.

Course description and syllabus:
Description: The objective of this course is to provide students with a working knowledge of classical molecular simulations. The theory and important concepts of molecular simulations will be covered. The students will write molecular dynamics and Monte Carlo codes and perform analysis.

Syllabus:
1. Review of Basic Concepts: Theory of Statistical Mechanics, Intermolecular Interactions and Potential Energy Surfaces

2. Molecular dynamics: Microcanonical and other ensembles, constrained simulations, non-equilibrium approaches, how to analyze results (radial distribution functions, probability distribution, ensemble averages, autocorrelation functions, transport properties).
3. Monte Carlo Methods: Random walks and Markov chains, Metropolis algorithm in various ensembles, biased Monte Carlo schemes
4. Free energy estimations: Mapping phase diagrams, generating free energy landscapes, collective variables
5. Rare event simulations: Transition path sampling, forward flux sampling, umbrella sampling, meta-dynamics, weighted histogram methods.
6. Using available Molecular Simulations codes for different applications: LAMMPS, Gromacs, Protein-ligand docking packages.

Accommodations for Students with Disabilities: Any student who suspects s/he may need an accommodation based on the impact of a disability should contact the instructor privately as soon as possible (preferably by Jan. 22) to discuss specific needs *and provide written documentation from the Office of Student Accessibility Services*. If not yet registered as a student with a disability, please contact the Office of Student Accessibility Services at 740-593-2620, or visit the office in 348 Baker University Center.

Preferred Name and Pronoun Policy: Consistent with OHIO policy, the preferred name and pronoun will be used in lieu of the legal name when it is not necessary for the legal name to be used. Faculty, staff, and students are expected to facilitate the use of preferred name and pronoun.

Academic Conduct: Engineering is a profession, and ethical behavior is expected of professionals. You are expected to act in a professional manner in this course. Disrespect to any of the students in the class, the instructor, or TA will not be tolerated. If a student acts in such a manner, s/he will be asked to leave the classroom and will lose any credits for the activity that takes place that day (including exams). Academic dishonesty is defined in the *Student Handbook* and will be dealt with according to the guidelines therein. Also note that the Russ College has adopted an Honor Code, details of which can be accessed at http://www.ohio.edu/engineering/integrity/code/index.cfm. Exchanging information on assignments or exams where such an exchange has been forbidden and plagiarism are violations of the standards set forth in this course and the *Student Handbook* in general. Other violations include any action taken to gain an unfair advantage during exams (e.g., taking more time than allowed, bringing in non-permitted materials), any action that deliberately deceives your professor or your classmates, any action taken without due consideration of its possible harmful effect on others. Appropriate penalties will be imposed, which could include a zero on the assignment or exam, failing the course, and/or a referral to the Office of Judiciaries (refer to the *Student Handbook* for descriptions of unethical behavior and the potential penalties). University Judiciaries may impose additional sanctions. Students may appeal academic sanctions through the grade appeal process.

Mental and Emotional Wellbeing: College can be a stressful time, and many things can prevent you from performing at your best, including strained relationships, increased anxiety, alcohol/drug problems, feeling down, difficulty concentrating and/or lack of motivation. If you find yourself dealing with these or other issues that affect your mental health or academic performance, Ohio University offers services that can help. Counseling and Psychological Services provides drop-in counseling hours at Hudson Hall (3rd floor) from 9:45-3:15 Monday-Friday, as well as Counselor-in-Residence hours Sunday-Friday from 5-10 pm in Living Learning Center, Room 160. Services are free to students with guaranteed tuition or the Wellbeing Plan, and students can typically add

the Wellbeing Plan for a modest fee at any time in the term. If you need immediate assistance, you may call (740) 593-1616 24 hours per day, 7 days a week. For additional resources, visit https://www.ohio.edu/student-affairs/counseling.