

SYLLABUS – CHEM 537: APPLICATIONS IN COMPUTATIONAL CHEMISTRY

DATE LAST MODIFIED: 12/22/21

CREDITS: 3

TIME AND LOCATION: MWF 9:10 – 10AM, ROOM FUL 225

INSTRUCTOR: AURORA E. CLARK (FUL. 275)

OFFICE HOURS: UPON REQUEST

TEXTBOOK: CHRISTOPHER CRAMER “ESSENTIALS OF COMPUTATIONAL CHEMISTRY: THEORIES AND MODELS”

SUPPLEMENTAL TEXT: WILL BE PROVIDED AS NEEDED

ONLINE DOCUMENTATION THROUGH COURSE GITHUB

COURSE OVERVIEW: CHEM 537 FOCUSES PRIMARILY UPON LEARNING THE FUNDAMENTALS OF STATISTICAL MECHANICS SIMULATIONS OF CHEMICAL SYSTEMS. CLASSICAL MOLECULAR DYNAMICS METHODS AND SOFTWARE (LAMMPS AND GROMACS) WILL BE EMPHASIZED, WITH AB-INITIO MOLECULAR DYNAMICS (CP2K) AND MONTE CARLO METHODS DISCUSSED AS RELEVANT. SHELL SCRIPTING AND PYTHON ANALYSIS SKILLS WILL BE DEVELOPED TO ASSESS FUNDAMENTAL SYSTEM PROPERTIES.

COURSE SCHEDULE:

RED ITEMS – HOLIDAYS, MISSED CLASSES AND MAKEUP CLASSES

BLUE ITEMS – EXAMS, HW, OR QUIZZES

WEEK	DISCUSSION AND PROBLEM SOLVING TOPICS	NOTES
1 (1/10 - 1/14)	GETTING STUDENTS SET UP	GITHUB, KAMIAK, ETC HW#1 MOVING FILES, GITHUB PRACTICE
2 (1/17 - 1/21)	PACKMOL, AVOGADRO, INTRO TO MM	CREATING YOUR FIRST SIMULATION BOX
3 (1/24 - 1/28)	FORCE FIELDS AND ENERGY MINIMIZATION/OPTIMIZATION ROUTINES, PBC AND PME	HW#2 PLOTTING FF IN JUPYTER NOTEBOOKS , INPUT FILE STRUCTURE, SUBMISSION ON KAMIAK
4 (1/31 - 2/4)	ENSEMBLES AND THERMOMECHANICAL EQUILIBRATION	INTRO TO MD ALGORITHMS, THERMOSTATS AND BAROSTATS
5 (2/7 - 2/11)	ANALYZING OUTPUT FILES, USING VMD	HW #3, PLOTTING RDFs, ENERGIES, P, T, ETC.
6 (2/14 - 2/18)	MONTE CARLO ALGORITHMS	PROGRAMMING MC IN PYTHON

	PART I	
7 (2/21 - 2/25)	MC ALGORITHMS PART II	HW #4: SMALL MC PROGRAMMING CODE FOR AN ISING MODEL
8 (2/28 - 3/4)	PROJECT #1 UPDATES & DISCUSSION IN CLASS	FOR A SYSTEM GIVEN TO YOU, IDENTIFY CORRECT FORCE FIELD WITH JUSTIFICATION, IDENTIFY BENCHMARKS FOR VALIDATION, DEVELOP EQUILIBRATION PROTOCOL, EQUILIBRATE AND COMPARE DIFFERENT FORCE FIELDS OR EQUILIBRATION PROTOCOLS
9 (3/7 - 3/11)	FINISH PROJECT #1	TURN IN PROJECT #1
10 (3/14 - 3/18)	SPRING BREAK	
11 (3/24 - 3/18)	SPATIAL AND TEMPORAL CORRELATION FUNCTIONS IN MC AND MD	PRACTICING PROGRAMMING FUNCTIONS IN PYTHON
12 (3/21-3/25)	GRAPH THEORY ANALYSIS FOR MOLECULAR SIMULATIONS (MOLECULAR/INTRAMOLECULAR GRAPHS), DESCRIPTORS	HW #5: ANALYZE SPATIAL AND TEMPORAL CFs FROM PROJECT #1
13 (3/28 - 4/1)	TOPOLOGICAL DATA ANALYSIS AND HIERARCHICAL SPATIAL ORGANIZATION	APPLIED TO BINARY LJ FLUID,
14 (4/4 - 4/8)	PROJECT #2 DESIGN	HW #6: USE PYTHON TO A GRAPH REPRESENTATION AND THEN PERFORM MODULARITY OPTIMIZATION
15 (4/11 - 4/15)	PROJECT #2 UPDATES & CRITICAL THINKING OF SIMULATION LITERATURE PART I	HW #7 -STUDENTS WILL PROVIDE BRIEF UPDATES ON STATUS OF EQUILIBRATIONS AND ANALYSIS
16 (4/18 - 4/22)	CRITICAL THINKING OF SIMULATION LITERATURE PART II	HW#8, ASSIGNED READING WILL BE DISCUSSED LOOKING FOR HOLES/IMPROVEMENTS IN SIMULATION METHODOLOGY AND INTERPRETATION
17 (4/25 - 4/29)	PROJECT #2 PRESENTATIONS	

ASSIGNMENTS: THE HOMEWORK IS ASSIGNED AND DUE AT THE BEGINNING OF CLASS UNLESS OTHERWISE NOTED. HOMEWORKS WILL BE LARGELY DEMONSTRATION BASED AND SHARED VIA A GITHUB ACCOUNT FOR THE COURSE. THERE WILL BE TWO LARGE COURSE PROJECTS, ONE DUE AT

THE MID-TERM AND ONE AT THE END OF THE SEMESTER. THE FIRST COURSE PROJECT WILL DEMONSTRATE CORE SKILLS THAT INCLUDE SCRIPTING/ANALYSIS OF TEST SYSTEMS, WHILE THE SECOND PROJECT WILL BE TAILORED TO COMPLEMENT THE STUDENT'S CURRENT RESEARCH AREAS OF INTEREST.

GRADING

PARTICIPATION POINTS ASSESSED THROUGH HWS: 25%

PROJECT #1: 35 %

PROJECT #2: 40%

Class Policy on Late/Early Assignments: Late HW assignments may be turned in, with at 10% penalty for every late day being assessed on top of the actual HW score. HW assignments may be turned in early with no penalty.

Academic Integrity: Cheating or plagiarism in any form will not be tolerated. Cheating includes, but is not limited to: copying work or allowing your work to be copied; use of unauthorized material at quizzes and exams, any communication between students during a quiz or exam, and actively looking at another student's paper during a quiz or exam. Students repeating the course must rework and rewrite all assignments. Plagiarism includes resubmitting previously graded homework from a previous semester, even if they were your own work. Obtaining information about quizzes taken in prior semesters of this course is considered cheating. Use of any electronic device other than an approved calculator during a quiz or examination is cheating. All incidences of cheating will be reported to the Office of Student Affairs. The first incidence of cheating will result in a score of zero for that assignment, quiz or exam. A second incident of cheating will result in an F for the course and possible dismissal from the University.

Accommodations: Reasonable accommodations are available for students who have a documented disability. If you need accommodations to fully participate in this class, please visit the Access Center. All accommodations **MUST** be approved through the Access Center (Washington Bldg, Room 217). Please stop by or call 509-335-3417 to make an appointment with an Access Advisor. Further information is available at <http://accesscenter.wsu.edu>

COVID-19 STATEMENT

PER THE PROCLAMATION OF GOVERNOR INSLEE ON AUGUST 18, 2021, MASKS THAT COVER BOTH THE NOSE AND MOUTH MUST BE WORN BY ALL PEOPLE OVER THE AGE OF FIVE WHILE INDOORS IN PUBLIC SPACES. THIS INCLUDES ALL WSU OWNED AND OPERATED FACILITIES. THE STATE-WIDE MASK MANDATE GOES INTO EFFECT ON MONDAY, AUGUST 23, 2021, AND WILL BE EFFECTIVE UNTIL FURTHER NOTICE.

PUBLIC HEALTH DIRECTIVES MAY BE ADJUSTED THROUGHOUT THE YEAR TO RESPOND TO THE EVOLVING COVID-19 PANDEMIC. DIRECTIVES MAY INCLUDE, BUT ARE NOT LIMITED TO, COMPLIANCE WITH WSU'S COVID-19 VACCINATION POLICY, WEARING A CLOTH FACE COVERING, PHYSICALLY DISTANCING, AND SANITIZING COMMON-USE SPACES. ALL CURRENT COVID-19 RELATED UNIVERSITY POLICIES AND PUBLIC HEALTH DIRECTIVES ARE LOCATED AT [HTTPS://WSU.EDU/COVID-19/](https://wsu.edu/covid-19/). STUDENTS WHO CHOOSE NOT TO COMPLY WITH THESE DIRECTIVES MAY BE REQUIRED TO LEAVE THE CLASSROOM; IN EGREGIOUS OR REPETITIVE CASES, STUDENT NON-COMPLIANCE MAY BE REFERRED TO THE CENTER FOR COMMUNITY STANDARDS FOR ACTION UNDER THE STANDARDS OF CONDUCT FOR STUDENTS.