



**MASC 575 Basics of Atomistic Simulation of
Materials**

Units: 4

Fall 2021

Time: Lecture: M/W, 4-5:50pm

Location: TBD

Instructor: Ken-ichi Nomura

Office: VHE 609

Office Hours: TBD

Contact Info: knomura@usc.edu

Teaching Assistant: TBD

Office Hours: TBD

Contact Info: TBD

Course Description

This course introduces basics of atomistic simulation methods with special focuses on Molecular Dynamics (MD) and Monte Carlo (MC) simulations. Due to the rapid advances of high-performance parallel computers, atomistic simulation has become an essential tool to investigate material structures and properties. The course provides overview of atomistic simulations, their applications, underlying theory and algorithms. Hands-on projects using the USC Advanced Research Computing supercomputer develops solid understanding of how to design and perform materials simulations. This course is designed for graduate students with any science and engineering background. No prior experience of programming is necessary.

Learning Objectives

In this course, students will learn materials modeling and simulations in order to:

1. Develop solid understanding of basic concepts and algorithms in atomistic materials modeling.
2. Understand how to characterize and study materials properties.
3. Design and perform atomistic simulations on the USC CARC computers.

Prerequisite(s): None

Recommended Preparation: None

Course Notes

Grading type: letter grade. All course notes will be provided on Blackboard.

Technological Proficiency and Hardware/Software Required

Personal laptop computer is necessary to access the HPC server and work on the projects. Students will be provided materials simulation programs and individual HPC account for the projects.

Recommended Readings and Supplementary Materials

Understanding Molecular Simulation – From Algorithm to Applications by Frenkel and Smit (ISBN-13: 978-0122673511)

Reading materials will be given in the class and posted on Blackboard.

Description and Assessment of Assignments

The learning outcome is assessed by four tests, two projects, and final project review. One test will be given roughly every month (four tests in total) on topics covered in the lectures during each period. MC and MD projects provides solid understanding and hands-on experiences of the simulation methodologies. During the final week each student will meet with instructor to go through project reports, discuss the subject, and be given comments and feedbacks.

Grading Breakdown

Assignments	Points	% of Grade
Homework	20	20%
Exams	30	30%
Projects	50	50%
Total	100	100%

Assignment Submission Policy

MC project due is in two weeks and MD project is due in four weeks.

Grading Timeline

Each test will be graded within two weeks. The grade will be posted on Blackboard.

Course Schedule Breakdown

- **Introduction:** Course Overview & HPC Account Setup
- **MD Basics:** Interatomic Potential, Numerical Discretization, Force Derivation
- **Time Integrators:** Verlet and velocity-Verlet algorithms
- **Initial and Boundary Conditions:** PBC and MIC, crystal structures
- **Atomic Velocities:** Probability Density Functions and Transformation of Coordinates
- **Canonical ensemble:** Partition Function, Mean and Fluctuation, Specific Heat
- **Ensemble Method:** Lagrangian and Hamiltonian Dynamics, Isothermal and Isobaric ensembles, Applications of Ensemble Methods
- **Hands-on :** Linux, High-performance Computing, Fortran Programming, MC and MD projects

Statement on Academic Conduct and Support Systems

Academic Conduct:

Plagiarism – presenting someone else’s ideas as your own, either verbatim or recast in your own words – is a serious academic offense with serious consequences. Please familiarize yourself with the discussion of plagiarism in SCampus in Part B, Section 11, “Behavior Violating University Standards” policy.usc.edu/scampus-part-b. Other forms of academic dishonesty are equally unacceptable. See additional information in SCampus and university policies on scientific misconduct, policy.usc.edu/scientific-misconduct.

Support Systems:

Counseling and Mental Health - (213) 740-9355 – 24/7 on call
studenthealth.usc.edu/counseling

Free and confidential mental health treatment for students, including short-term psychotherapy, group counseling, stress fitness workshops, and crisis intervention.

National Suicide Prevention Lifeline - 1 (800) 273-8255 – 24/7 on call

suicidepreventionlifeline.org

Free and confidential emotional support to people in suicidal crisis or emotional distress 24 hours a day, 7 days a week.

Relationship and Sexual Violence Prevention and Services (RSVP) - (213) 740-9355(WELL), press "0" after hours – 24/7 on call

studenthealth.usc.edu/sexual-assault

Free and confidential therapy services, workshops, and training for situations related to gender-based harm.

Office of Equity and Diversity (OED)- (213) 740-5086 | Title IX – (213) 821-8298

equity.usc.edu, titleix.usc.edu

Information about how to get help or help someone affected by harassment or discrimination, rights of protected classes, reporting options, and additional resources for students, faculty, staff, visitors, and applicants. The university prohibits discrimination or harassment based on the following *protected characteristics*: race, color, national origin, ancestry, religion, sex, gender, gender identity, gender expression, sexual orientation, age, physical disability, medical condition, mental disability, marital status, pregnancy, veteran status, genetic information, and any other characteristic which may be specified in applicable laws and governmental regulations. The university also prohibits sexual assault, non-consensual sexual contact, sexual misconduct, intimate partner violence, stalking, malicious dissuasion, retaliation, and violation of interim measures.

Reporting Incidents of Bias or Harassment - (213) 740-5086 or (213) 821-8298

usc-advocate.symplicity.com/care_report

Avenue to report incidents of bias, hate crimes, and microaggressions to the Office of Equity and Diversity | Title IX for appropriate investigation, supportive measures, and response.

The Office of Disability Services and Programs - (213) 740-0776

dsp.usc.edu

Support and accommodations for students with disabilities. Services include assistance in providing readers/notetakers/interpreters, special accommodations for test taking needs, assistance with architectural barriers, assistive technology, and support for individual needs.

USC Support and Advocacy - (213) 821-4710

uscsa.usc.edu

Assists students and families in resolving complex personal, financial, and academic issues adversely affecting their success as a student.

Diversity at USC - (213) 740-2101

diversity.usc.edu

Information on events, programs and training, the Provost's Diversity and Inclusion Council, Diversity Liaisons for each academic school, chronology, participation, and various resources for students.

USC Emergency - UPC: (213) 740-4321, HSC: (323) 442-1000 – 24/7 on call

dps.usc.edu, emergency.usc.edu

Emergency assistance and avenue to report a crime. Latest updates regarding safety, including ways in which instruction will be continued if an officially declared emergency makes travel to campus infeasible.

USC Department of Public Safety - UPC: (213) 740-6000, HSC: (323) 442-120 – 24/7 on call

dps.usc.edu

Non-emergency assistance or information.