The University of Texas at Austin
Department of Chemical Engineering

ChE 384T: Computational Methods in Materials Science

UNIQUE #: 15755, FALL 2024

CLASS TIMES: 09:00 am – 10:00 am on Mondays, Wednesdays, and Fridays in CPE 2.222

Instructor: Wennie Wang

Office: CPE 4.450
Office hours: by appointment
Email:wwwennie@che.utexas.edu
Phone: 512-471-9894
Pronouns: she/her/hers

Course Description

This course is an introductory survey to simulation techniques used in materials science for modeling materials phenomena. The emphasis of this course is on developing a mathematical, algorithmic, and physical understanding for materials simulation. The methods covered in this course will be connected to several on-going research areas and technological applications in chemical engineering and materials science.

By the end of this course, students will be expected to be able to:

- Implement materials modeling methods using basic principles and concepts of scientific coding
- Generate, analyze, and visualize simulated data
- Interpret simulate data and explain its physical significance
- Propose physical models for modeling complex materials phenomena, identify their assumptions and limitations, and suggest improvements to the simulation
- Communicate (oral and written) their results to a general audience

The course will be based on Python, a popular open-source programming language in materials science.

Prerequisites: graduate standing or consent of instructor.

Course materials

Main text: Richard Lesar. *Introduction to Computational Materials Science.* 2013. https://doi.org/10.1017/CBO9781139033398; ISBN: 9780521845878

Course Outline

All instructions, assignments, readings, rubrics and essential information will be on the Canvas website at utexas.instructure.com. Any changes to the course and announcements will be made on Canvas in as much advance time as possible. **Please be sure to check Canvas regularly.**

Course Requirements and Grading

Coursework: This course will consist of keeping up with reading, ~5-6 homework assignments, and a final project (proposal, code, report, and presentation).

Background expectations:
No background in scientific programming is assumed. Students are expected to have a basic familiarity with:

- scientific units conversions
- trigonometric, exponential, logarithm, polynomial functions
- matrix operations (e.g., addition, multiplication)
- concepts in statistics and probability
- multivariate derivatives and integrals

Course devices:

- Computer or work station with the following minimum specifications: 2 GB RAM (4 GB preferred), relatively modern OS (e.g., Windows 7 or Ubuntu 16.04)
- Word processor, an IDE, latest version of Python (if you prefer another programming language, please inform the instructor first)

You will also want access to a computer and a reliable internet connection. If you have difficulties with access to either, please inform the instructor as soon as possible.

Course mode: Face-to-face unless otherwise specified. Lecture materials will be made available on Canvas as announced.

GRADES

Coursework Breakdown:

- Homework (50%): upload to Canvas by the deadline indicated. **Late work:** This course will have a relatively heavy component of peer review. As such, it is highly recommended to submit by the deadline. If you anticipate a submission delay or require an extension, please arrange ahead of time with the instructor.
- Peer participation (25%): surveys, class discussion, in-class activities
- Final Project (5% proposal, 10% report, 10% presentation): upload to Canvas by the deadlines indicated

Grade breakdown:
> 90% (A), 88-89% (A-), 82-87% (B+), 75-82% (B), 71-75% (B-), 68-71% (C+), 58-68% (C), 55-58% (C-), 50-55% (D), < 50% (F)

LECTURE TOPICS

* Readings and supplementary materials may also be posted

* Subject to change

^ = time permitting

Class Topic	Reading (LeSar)	Notes
Introduction to materials modeling and simulation	Ch. 1, Appendix A	
A brief introduction to crystallography	Appendix B1-B5	
Random Walk Diffusion	Ch. 2, Appendix B7, C5, I2-I3	PS1, see also Ch. 8
Simulation of finite systems	Ch. 3	PS2
Interatomic potentials	Ch. 5, Appendix D4	PS3
Molecular dynamics	Ch. 6, Appendix I4	PS4
Molecular dynamics and connection to stat mech	Appendix G	
Monte Carlo	Ch. 7, Appendix C4, D1-D4	PS5
Kinetic Monte Carlo	Ch. 9	
Monte Carlo at the mesoscale	Ch. 10	
Cellular Automata^	Ch. 11	
Electronic Structure methods^	Ch. 4, Appendix F	
Machine learning in materials science^	Ch. 14	

Coding Resources

Free, no account needed:

- Tutorials from the official documentation: https://docs.python.org/3/tutorial/index.html
- LearnPython.org: https://www.learnpython.org/
- Automate the Boring Stuff: https://automatetheboringstuff.com/
- FreeCodeCamp.org (4 hr Youtube video): https://www.youtube.com/watch?v=rfscVS0vtbw
- Google for Education: https://developers.google.com/edu/python

Free, account needed:

- Udemy: https://www.udemy.com/course/pythonforbeginnersintro/
- Microsoft: https://learn.microsoft.com/en-us/training/modules/intro-to-python/

Other useful resources

- LaTeX (document, type-setting software)
- Overleaf (online LaTeX editor)

Course Policies

OFFICE HOURS

Office hours are open-door policy, meaning you are welcome to discuss topics including and beyond the course material (e.g., career advice, doing research). Please come by! Office hours may be in-person or remote, as announced on Canvas.

Please also let Prof. Wang know if you have any announcements you would like advertised at the start of class (e.g., student org events, general useful knowledge).

COLLABORATING ON HOMEWORKS

You are allowed (and in fact, encouraged) to collaborate (i.e., discuss, brainstorm) with your classmates in small groups (~3-5) on the homework. The work you turn in must entirely reflect your own work (e.g., you may not simply copy each other's answers). If you choose to collaborate, please list the names of the people you worked with for that particular assignment at the top of the first page.

ACADEMIC INTEGRITY EXPECTATIONS

You are expected to uphold all standards of academic integrity described in the University Code of Conduct and the Student Honor Code.

Students who violate University rules on academic dishonesty are subject to disciplinary penalties, including the possibility of failure in the course and/or dismissal from the University. Since such dishonesty harms the individual, all students, and the integrity of the University, policies on academic dishonesty will be strictly enforced.

For further information, please visit the Student Conduct and Academic Integrity website at: http://deanofstudents.utexas.edu/conduct.

USE OF CHATGPT

The use of ChatGPT is permitted but any work submitted must reflect the effort and understanding of the student. To get the most out of the course, students are encouraged to take the time to understand and critically evaluate the output. ChatGPT is a generative language learning model. As such, ChatGPT is not always capable of producing reliable or truthful statements. Nevertheless, it can provide a useful starting point when prompted appropriately.

For additional guidelines and ideas, see e.g., Buriak et al. “Best Practices for Using AI When Writing Scientific Manuscripts.” *ACS Nano* editorial. Feb 27, 2023. https://pubs.acs.org/doi/10.1021/acsnano.3c01544

LECTURE ONLINE

This class is using the Lectures Online recording system. This system records the audio and video material presented in class for you to review after class. Links for the recordings will appear in the Lectures Online tab on the Canvas page for this class. You will find this tab along the left side navigation in Canvas.

To review a recording, simply click on the Lectures Online navigation tab and follow the instructions presented to you on the page. You can learn more about how to use the Lectures Online system at http://sites.la.utexas.edu/lecturesonline/students/how-to-access-recordings/.

You can find additional information about Lectures Online at: https://sites.la.utexas.edu/lecturesonline/.

CONFIDENTIALITY OF CLASS RECORDINGS

Class recordings are reserved only for students in this class for educational purposes and are protected under FERPA. The recordings should not be shared outside the class in any form. Violation of this restriction by a student could lead to Student Misconduct proceedings.

SHARING OF COURSE MATERIALS IS PROHIBITED

No materials used in this class, including, but not limited to, lecture hand-outs, videos, assessments (quizzes, exams, papers, projects, homework assignments), in-class materials, review sheets, and additional problem sets, may be shared online or with anyone outside of the class without explicit, written permission of the instructor. Unauthorized sharing of materials promotes cheating. The University is well aware of the sites used for sharing materials, and any materials found online that are associated with you, or any suspected unauthorized sharing of materials, will be reported to Student Conduct and Academic Integrity in the Office of the Dean of Students. These reports can result in sanctions, including failure of the course.

GETTING HELP WITH TECHNOLOGY

Students needing help with technology in this course should contact the ITS Service Desk.University Resources for Students

SERVICES FOR STUDENTS WITH DISABILITIES (SSD)

I am committed to creating an accessible and inclusive learning environment in this class. Please let me know if you experience any barriers to learning so I can work with you to ensure you have equal opportunity to participate fully in this course. If you are a student with a disability, or think you may have a disability, and need accommodations please contact Services for Students with

Disabilities (SSD). Please refer to SSD's website for contact and more information: http://diversity.utexas.edu/disability/.

If you are already registered with SSD, please discuss with and/or deliver your Accommodation Letter to Prof. Wang at the start of the semester your accommodations and needs in this course.

COUNSELING AND MENTAL HEALTH CENTER (CMHC)

If you or anyone you know is experiencing symptoms of stress, anxiety, depression, academic concerns, loneliness, difficulty sleeping, or any other concern impacting your well-being – you are strongly encouraged to connect with CMHC. The Counseling and Mental Health Center provides a wide variety of mental health services to all UT students including crisis services, counseling services with immediate support and well-being resources. Additionally, CARE Counselors are located within the academic schools and colleges. These counselors get to know the concerns that are unique to their college's students. For more information on CMHC, visit https://cmhc.utexas.edu or call 512-471-3515.

Important Safety Information

If you have concerns about the safety or behavior of fellow students, TAs or professors, contact BCCAL (the Behavior Concerns and COVID-19 Advice Line) at https://safety.utexas.edu/behavior-concerns-advice-line or by calling 512-232-5050. Confidentiality will be maintained as much as possible, however the university may be required to release some information to appropriate parties.

CLASSROOM SAFETY AND COVID-19

To help preserve our in-person learning environment, please consider the following:

- Adhere to university mask guidance. Masks are strongly recommended inside university buildings for vaccinated and unvaccinated individuals.
- Vaccinations are widely available, free and not billed to health insurance. The vaccine will help protect against the transmission of the virus to others and reduce serious symptoms in those who are vaccinated.
- Proactive Community Testing remains an important part of the university's efforts to protect our community. Tests are fast and free.
- We encourage the use of the Protect Texas App each day prior to coming to campus.
- If you develop COVID-19 symptoms or feel sick, stay home and contact the University Health Services' Nurse Advice Line at 512-475-6877. If you need to be absent from class, contact Student Emergency Services and they will notify your professors. In addition, to help understand what to do if you have been had close contact with someone who tested positive for COVID-19, see University Health Services link.
- Behavior Concerns and COVID-19 Advice Line (BCCAL) remains available as the primary tool to address questions or concerns from the university community about COVID-19.
- Students who test positive should contact BCCAL or self-report (if tested off campus) to University Health Services.
- Visit Protect Texas Together for more information.

TITLE IX DISCLOSURE

Beginning January 1, 2020, TexasSenate Bill 212 requires all employees of Texas universities, including faculty, to report any information to theTitle IX Office regarding sexual harassment, sexual assault, dating violence and stalking that is disclosed to them. Texas law requires that all employees who witness or receive any information of this type (including, but not limited to, writing assignments, class discussions, or one-on-one conversations) must be reported. If you would like to speak with someone who can provide support or remedies without making an official report to the university, please email advocate@austin.utexas.edu. For more information about reporting options and resources, visit http://www.titleix.utexas.edu/, contact the Title IX Office via email at titleix@austin.utexas.edu, or call 512-471-0419. Although graduate teaching and research assistants are not subject to Texas Senate Bill 212, they are still mandatory reporters under Federal Title IX laws and are required to report a wide range of behaviors we refer to as sexual misconduct, including the types of sexual misconduct covered under Texas Senate Bill 212.The Title IX office has developed supportive ways to respond to a survivor and compiled campus resources to support survivors.

Faculty members and certain staff members are considered “Responsible Employees” or “Mandatory Reporters,” which means that they are required to report violations of Title IX to the Title IX Coordinator. **I am a Responsible Employee and must report any Title IX-related incidents** that are disclosed in writing, discussion, or one-on-one. Before talking with me or with any faculty or staff member about a Title IX-related incident, be sure to ask whether they are a responsible employee. If you want to speak with someone for support or remedies without making an official report to the university, email advocate@austin.utexas.edu For more information about reporting options and resources, visit the Title IX Office or email titleix@austin.utexas.edu.