UW-Madison Syllabus Template

1 Course Subject, Number and Title

MSE760: Molecular Modeling in Materials (Previously: Molecular Dynamics and Monte Carlo Simulations in Materials Science)

2 Credits

3 credits, contact hours = 150min/wk (consistent with credit hours requirements specified in Sec. 8).

3 Course Designations and Attributes

None (I don't think – need to check this).

4 Course Description

This course will provide students with hands-on experience in modern tools of solid state and molecular modeling, including quantum mechanical simulations, molecular dynamics, and Monte-Carlo approaches for material sciences. We will also include some select additional/advanced techniques like beyond mean-field electronic structure theory, quantum mechanical calculations of magnetism, spectroscopic, and transport properties for solids and condensed phases, as well as machine-learning techniques.

The course will be application oriented, with a goal of learning to effectively use tools at an advanced level.

5 Requisites

None.

6 Meeting Time and Location

Tue./Thur. 9:30AM - 10:45AM
MECH ENGR 2106

7 Instructional Modality

In-person.

8 How Credit Hours are Met by the Course

Traditional Carnegie Definition – 1.25 hour (75 mins) of classroom or direct faculty/instructor instruction and a minimum of two hours of out of class student work each week over approximately 15 weeks, or an equivalent amount of engagement over a different number of weeks. This is the status quo and represents the traditional college credit format used for decades. If you have regular classroom meetings and assign homework, reading, writing, and preparation for quizzes and exams, make this choice.

9 Regular and Substantive Student-Instructor Interaction

This course engages students in teaching, learning and assessment through direct instruction, providing feedback on student work, and facilitating discussion of course content. Regular interaction includes class times.

10 Other Course Information

None.

11 Instructors & Teaching Assistants

None at present but may have some help from graduate students and postdocs in my lab.

1.1 Instructor Title and Name

Professor Yuan Ping (just call me Yuan).

1.2 Instructor Availability

Office hours will be conducted MSE 3104 (my office) Monday 5pm

1.3 Instructor Email/Preferred Contact

yping3@wisc.edu

1.4 Teaching Assistant (if applicable)

None at present.

1.5 TA Office Hours

None

1.6 TA Email/Preferred Contact

None

12 Course Learning Outcomes

Choose and use the appropriate molecular simulations to obtain properties of materials.
Apply ab initio methods to model materials properties.
Apply molecular dynamics methods to model materials properties.
Understand implications of results of molecular simulations in scientific literature.
Use molecular simulations to analyze a scientific or engineering problems to obtain selected insights and communicate them at a basic level. [UG]
Use molecular simulations to analyze a scientific or engineering problems to obtain selected insights and communicate them at a semi-professional level. [Grad]

Through this course, the students will learn the concepts of numerical computing for materials from the fundamental level to practical applications of important material properties regularly measured in the experimental labs. The course will focus on building the bridge of theory, numerical simulations and applications, understanding how to set up and perform calculations properly with existing codes. Students will learn Linux usage, massive-parallel calculations on HPC computers (optional), and programming for postprocessing analysis with student-preferred computing languages. This course is necessary for students who are interested in materials simulations for both predicting physical/chemical properties and interpreting experiments. Therefore, it is useful for both theorists who plan to work on computational materials and experimentalists who need helps for data interpretation.

13 Grading

- ~4 Quizzes (20%), ~4 labs (40%), Project (40%)
- Quizzes are graded automatically. Other assignments graded by instructor or grader.
- Grades may be curved depending on the overall mean of the class.
- Attendance is strongly encouraged but not formally graded. However, strong attendance can influence a borderline grade.
- Grading is an A-F scale.
- Requirements for each grade are below
    - A: Excellent performance on all measures (93-100).
    - AB: Minor lapses in performance in some areas (87-92).
    - B: Good average performance across all areas (83-86).
    - BC: Poor performance in some areas (77-82).
    - C: Poor performance in most areas (70-76).
    - D: Very poor performance in most areas (60-69).
    - F: Unacceptably poor performance in most areas (<60).

The numerical boundaries are based on standard ranges[1] and the instructor may move the grade boundaries depending on the overall mean of the class.

14 Course Website, Learning Management System & Digital Instructional Tools

Canvas: https://canvas.wisc.edu/courses/424256
Google docs: https://drive.google.com/drive/u/1/folders/1S8Pi4gc3EHII6pF3XH0PR2hPkgHsBjl_

15 Discussion Sessions (in-person or remote)

TBD

16 Laboratory Sessions (in-person or remote)

None (computational labs will be done during some class times)

17 Required Textbook, Software & Other Course Materials

None

Useful books (but not required). I will try to provide key readings as needed.

- Frenkel and Smit, Understanding Molecular Simulation, From Algorithms to Applications, 2nd Ed (Academic Press, 2001), ISBN-13: 978-0122673511 (Molecular Dynamics, Monte Carlo).
- R. Lesar, Computational Materials Science: Fundamentals to Applications (Cambridge University Press, 2013) (UW online access https://ebookcentral.proquest.com/lib/wisc/detail.action?docID=1139555) (Basic introductory book to many materials simulation methods).
- Electronic Structure (Basic Theory and Practical Methods)
  Richard Martin, University of Illinois, Urbana-Champaign, Cambridge University Press
- D. Sholl, J.A. Steckel, *Density functional theory: a practical introduction*. (Wiley-Interscience, 2009) (Density functional theory).

[1] https://en.wikipedia.org/wiki/Academic_grading_in_the_United_States

18 Homework & Other Assignments

The course is set up as Modules and Projects

1. Modules
    a. Introductory Topics (one week)
    b. Quantum Mechanics I (two weeks)
    c. Quantum Mechanics II (two weeks)
    d. Quantum Mechanics III (two weeks)
    e. Molecular Dynamics and Monte Carlo (three weeks)
    f. Machine Learning (two weeks)
2. Projects (reports, 3 weeks)

Each module typically (although not always) has

1. Quiz with 3 or more questions to assess very basic learning.
2. Lab.
3. Lectures.

Projects description is here:

Will come soon..

All quizzes given through Canvas.
All assignments are to be submitted through Canvas.
All class files delivered through gdocs.

19 Campus Spaces for Virtual Learning & Testing

Dedicated on-campus spaces with high-speed internet are available for students to reserve for any exam/quiz taken during the semester. Computers can also be requested. See https://virtuallearning.wisc.edu/ .

20 Exams, Quizzes, Papers & Other Major Graded Work

- Quizzes are at home, closed book (honor system), and timed at 10-30min. ~10 questions per quiz, worth 1 pt each. Labs are graded out of 10 points. Projects are graded out of 10 points. I may update this as the semester progresses.
- Deadlines for all assignments are in canvas calendar.
- Late assignments get (this is not usually necessary to enforce – just talk to me about late assignments in advance)
    - Labs: up to -2 points (20%) (-1 per day) until solution posted, then potentially 0.
    - Projects: -2 for any lateness.
- No exams.

21 Privacy of Student Information & Digital Tools: Teaching & Learning Analytics & Proctoring Statement

The privacy and security of faculty, staff and students' personal information is a top priority for UW-Madison. The university carefully reviews and vets all campus-supported digital tools used to support teaching and learning, to help support success through learning analytics, and to enable proctoring capabilities. UW-Madison takes necessary steps to ensure that the providers of such tools prioritize proper handling of sensitive data in alignment with FERPA, industry standards and best practices.

Under the Family Educational Rights and Privacy Act (FERPA which protects the privacy of student education records), student consent is not required for the university to share with school officials those student education records necessary for carrying out those university functions in which they have legitimate educationl interest. 34 CFR 99.31(a)(1)(i)(B). FERPA specifically allows universities to designate vendors such as digital tool providers as school officials, and accordingly to share with them personally identifiable information from student education records if they perform appropriate services for the university and are subject to all applicable requirements governing the use, disclosure and protection of student data.

22 Privacy of Student Records & the Use of Audio Recorded Lectures

Summary: Please don't make or share recorded materials outside of class.

See information about privacy of student records and the usage of audio-recorded lectures.
Lecture materials and recordings for this course are protected intellectual property at UW-Madison. Students in this course may use the materials and recordings for their personal use related to participation in this class. Students may also take notes solely for their personal use. If a lecture is not already recorded, you are not authorized to record my lectures without my permission unless you are considered by the university to be a qualified student with a disability requiring accommodation. [Regent Policy Document 4-1] Students may not copy or have lecture materials and recordings outside of class, including posting on internet sites or selling to commercial entities. Students are also prohibited from providing or selling their personal notes to anyone else or being paid for taking notes by any person or commercial firm without the instructor's express written permission. Unauthorized use of these copyrighted lecture materials and recordings constitutes copyright infringement and may be addressed under the university's policies, UWS Chapters 14 and 17, governing student academic and non-academic misconduct.

23 How to Succeed in This Course

1. Start early to complete tasks as it is easy to get stuck and need help (e.g., labs, quiz preparation, project work). A little help can save you many many hours but may not be available for a few days.
2. Start projects early and work steadily.
3. Use class discussion to develop a personalized understanding of the material.

24 Course Evaluations

I strongly encourage unsolicited feedback at any time to help make the course better. This is a new course and we are all learning how to make it most effective. I may also solicit feedback as a survey part way through the semester.

UW-Madison now uses an online course evaluation survey tool, AEFIS. In most instances, you will receive an official email two weeks prior to the end of the semester when your course evaluation is available. You will receive a link to log into the course evaluation with your NetID where you can complete the evaluation and submit it, anonymously. Your participation is an integral component of this course, and your feedback is important to me. I strongly encourage you to participate in the course evaluation.

25 Students' Rules, Rights & Responsibilities

During the global COVID-19 pandemic, we must prioritize our collective health and safety to keep ourselves, our campus, and our community safe. As a university community, we must work together to prevent the spread of the virus and to promote the collective health and welfare of our campus and surrounding community.

26 Diversity & Inclusion Statement

Diversity is a source of strength, creativity, and innovation for UW-Madison. We value the contributions of each person and respect the profound ways their identity, culture, background, experience, status, abilities, and opinion enrich the university community. We commit ourselves to the pursuit of excellence in teaching, research, outreach, and diversity as inextricably linked goals. The University of Wisconsin-Madison fulfills its public mission by creating a welcoming and inclusive community for people from every background – people who as students, faculty, and staff serve Wisconsin and the world.

27 Academic Integrity Statement

By virtue of enrollment, each student agrees to uphold the high academic standards of the University of Wisconsin-Madison; academic misconduct is behavior that negatively impacts the integrity of the institution. Cheating, fabrication, plagiarism, unauthorized collaboration, and helping others commit these previously listed acts are examples of misconduct which may result in disciplinary action. Examples of disciplinary action include, but is not limited to, failure on the assignment/course, written reprimand, disciplinary probation, suspension, or expulsion.

28 Accommodations for Students with Disabilities Statement

The University of Wisconsin-Madison supports the right of all enrolled students to a full and equal educational opportunity. The Americans with Disabilities Act (ADA), Wisconsin State Statute (36.12), and UW-Madison policy (Faculty Document 1071) require that students with disabilities be reasonably accommodated in instruction and campus life. Reasonable accommodations for students with disabilities is a shared faculty and student responsibility. Students are expected to inform faculty [me] of their need for instructional accommodations by the end of the third week of the semester, or as soon as possible after a disability has been incurred or recognized. Faculty [I], will work either directly with the student [you] or in coordination with the McBurney Center to identify and provide reasonable instructional accommodations. Disability information, including instructional accommodations as part of a student's educational record, is confidential and protected under FERPA. (See: McBurney Disability Resource Center)

29 Academic Calendar & Religious Observances

See: https://secfac.wisc.edu/academic-calendar/#religious-observances