ME/MSE 598 DM: Introduction to Digital Materials

Spring 2025

Schedule

TR 11:00–12:20 in 2051 Sidney Lu Mech. Eng. Building

Course content

- Reading: Google Drive shared folder, articles / e-books through library.illinois.edu
- Assignment upload: my.matse.illinois.edu/courses/upload, select MSE 598
- Course website: courses.grainger.illinois.edu/MSE598DM; PDF syllabus
- Juypter notebooks: Google Colab

Scope

- Introduction to the connection of materials and data science
- Specific issues regarding experimental and computational materials data
- Data acquisition and management, data curation
- Uncertainty quantification
- Applying machine learning to materials data

Objectives

Students will be able to

(a) critically review the scientific literature;
(b) apply your knowledge to answer scientific questions related to materials and data science;
(c) apply data science and machine learning to materials data;
(d) use materials data as a driver for materials design and discovery;
(e) explain their reasoning to their colleagues in small and large settings;
(f) work together with their colleagues in a professional, scientific manner.

Prerequisites

- Materials Science
  - Structure of materials; Properties of materials; Materials Characterization
- Computer Science

  - Programming and data structures; Programming experience (Python, C, C++, MATLAB)
- Mathematics
  - Linear algebra; Statistics

Instructor

Dallas R. Trinkle (dtrinkle@illinois.edu; 308 MSEB in the west stairwell).

- Professor and Associate Head (joined Univ. Illinois in 2006)
- Computational materials science
  - Crystalline defects (dislocations, point defects, interfaces) from density functional theory
  - Development of new algorithms, computational tools, materials models
  - Solid solution softening / strengthening, pipe diffusion, general theory of diffusion

Teaching approach: Hands-on project-based learning

An "active learning" approach where we focus on the course objectives: *applying knowledge to answer scientific questions about materials and data* and *critically engaging with the scientific literature*. You will:

- **Prepare** individually for class (reading papers, background literature, working out conceptual questions);
- **Apply** data science and machine learning to materials data
- **Discuss** your questions and deeper points with me and your colleagues;
- **Assess** the literature and discuss with your classmates.

Team-based learning: Team basics[1]

First off: Teams are not easy.

As you will find out, group work is not always easy. Team members sometimes cannot prepare for or attend group sessions because of other responsibilities, and conflicts often result from differing skill levels and work ethics. When teams work and communicate well, however, the benefits more than compensate for the difficulties. Chances of success are greatly improved with some structure.

- **F**acilitator: make sure that goals are all achieved
- **M**oderator: make sure that everyone's ideas are heard, finds resolutions
- **P**resenter: report experience / conclusion to the rest of class
- **S**cribe: screen share the response document to work collaboratively
- **D**evil's advocate: quality control (does the argument make sense?)

In addition, the real world, for the most part, requires people to work together and interface skills, etc. Teamwork is a highly valued skill, but like all skills, requires practice.

[1] Adapted from Prof. Richard Felder, NCSU.

Literature assessment[2]

One primary activity of our class is *engaging actively with scientific literature*. This is a primary activity for scientists, and is a skill. It requires

- Reading primary papers, and the papers' bibliography.
- Working through background reading to build understanding.
- Discussing with others to test your understanding.
- Come to a judgment about:
  - What has been done well/poorly;
  - What might be done in the future;
  - What are the outstanding questions?

The focus will be on current scientific literature in the emerging materials and data area.

Minute paper

From time to time, we will conclude with a **minute paper** which helps to synthesize your understanding of the lecture, think about your questions, and prime discussion for the next class period. This will be done electronically using the link: forms.illinois.edu/sec/4555495. There, you will have three questions:

1. What are the two (or more) most significant (central, useful, meaningful, surprising) things you have learned during this lecture?
2. What main question(s) remain for you?
3. Is there anything that you did not understand?

Following class, I will compile the questions, organize them, and answer some of them online (on the course website). Your responses also help me to adjust the course as needed.

Grading

Each unit, noted below in the schedule, will involve hands-on sessions. You will turn in a PDF report on each of your hands on activities. The report should include a narrative about what you are doing and why. Learning how to do this is an important part of doing science.

Formal and Informal Accommodations

I am committed to assisting students requiring special accommodations for circumstances that are registered with the DRES Student Services Department. These formal accommodations should be discussed with me as early as possible in the semester or as soon after DRES approval as possible.

If you are not formally registered with DRES and have anxiety, depression, learning disabilities, or other issues that affect your ability to fully participate and learn in this class, you are encouraged to check-in with me so we can determine together the kind of support you need to thrive in this class. Please set up a meeting with me via email.

[2]This is what your advisor and future employers (academic, labs, industry) will expect you to be able to do after you graduate.

Inclusion and Diversity

I value all students regardless of their background, race, religion (creed), ethnicity, gender, gender expression, age, country of origin, disability status, marital status, sexual orientation, or military status, etc., and am committed to providing a climate of excellence and inclusiveness within all aspects of the course. If there are aspects of your culture or identity that you would like to share with me as they relate to your success in this class, I am happy to meet to discuss. Likewise, if you have any concerns in this area of facing any special issues or challenges, you are encouraged to discuss the matter with me (set up a meeting via email) with an assurance of full confidentiality (only exception being mandatory reporting of academic integrity / code violation and sexual harassment). **Harassment or discrimination of any kind will not be tolerated.**

Anti-Racism and Inclusivity Statement

The intent is to raise student and instructor awareness of the ongoing threat of bias and racism and of the need to take personal responsibility in creating an inclusive learning environment.

The Grainger College of Engineering is committed to the creation of an anti-racist, inclusive community that welcomes diversity along a number of dimensions, including, but not limited to, race, ethnicity and national origins, gender and gender identity, sexuality, disability status, class, age, or religious beliefs. The College recognizes that we are learning together in the midst of the Black Lives Matter movement, that Black, Hispanic, and Indigenous voices and contributions have largely either been excluded from, or not recognized in, science and engineering, and that both overt racism and micro-aggressions threaten the well-being of our students and our university community.

Learning Environment

The effectiveness of this course is dependent upon each of us to create a safe and encouraging learning environment that allows for the open exchange of ideas while also ensuring equitable opportunities and respect for all of us. Everyone is expected to help establish and maintain an environment where students, staff, and faculty can contribute without fear of personal ridicule, or intolerant or offensive language. If you witness or experience racism, discrimination, micro-aggressions, or other offensive behavior, you are encouraged to bring this to the attention of the course director if you feel comfortable. You can also report these behaviors to the Office of the Vice Chancellor for Diversity, Equity and Inclusion (OVCDEI). Based on your report, OVCDEI members will follow up and reach out to students to make sure they have the support they need to be healthy and safe. If the reported behavior also violates university policy, staff in the Office for Student Conflict Resolution may respond as well and will take appropriate action.

Religious Observances

Illinois law requires the University to reasonably accommodate its students' religious beliefs, observances, and practices in regard to admissions, class attendance, and the scheduling of examinations and work requirements. You should examine this syllabus at the beginning of the semester for potential conflicts between course deadlines and any of your religious observances. If a conflict

exists, you should notify your instructor of the conflict and follow the procedure at ODOS to request appropriate accommodations. This should be done in the first two weeks of classes.

Sexual Misconduct Reporting Obligation

The University of Illinois is committed to combating sexual misconduct. Faculty and staff members are required to report any instances of sexual misconduct to the University's Title IX Office. In turn, an individual with the Title IX Office will provide information about rights and options, including accommodations, support services, the campus disciplinary process, and law enforcement options.

A list of the designated University employees who, as counselors, confidential advisors, and medical professionals, do not have this reporting responsibility and can maintain confidentiality, can be found here: wecare.illinois.edu confidentiality.

Other information about resources and reporting is available here: wecare.illinois.edu.

Family Educational Rights and Privacy Act (FERPA)

Any student who has suppressed their directory information pursuant to Family Educational Rights and Privacy Act (FERPA) should self-identify to the instructor to ensure protection of the privacy of their attendance in this course. See FERPA info for more information on FERPA.

Academic Integrity

You are bound by the University Honor Code in this course. Any violation of the Honor Code will result in disciplinary action.

Students are responsible for producing their own code, reports, and projects. Collaborative interaction is encouraged, but each student must do their own implementation, perform all calculations themselves, and write their own reports. **Plagiarism will not be tolerated, and verified incidents will result in all parties receiving a zero and formal academic sanctions.** Students are responsible for familiarizing themselves with the definition of and penalties for plagiarism in Section I-401 of the UIUC Student Code. Note that plagiarism includes "copying another student's paper or working with another person when both submit similar papers without authorization to satisfy an individual assignment."

Changes to syllabus

May occur as deemed necessary by the professor; they will be announced and the updated syllabus posted on the course website.

Accessing files

The Univ. Illinois library has access to a huge variety of electronic resources; this plus additional online resources will be our references. Many can be accessed from the library's website, or via the campus VPN. Alternatively, you can take advantage of the library proxy. This is done by appending `proxy2.library.illinois.edu` to the web address; when reloaded, you will be asked for

Univ. Illinois authentication, and then will be able to access the resource as if you were on campus. In general, this authentication is required only once per session. So, the website

`http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.113.025504`

would become

`http://journals.aps.org.proxy2.library.illinois.edu/prl/abstract/10.1103/Phy`

Alternatively, install the Proxy Bookmarklet which makes it extremely easy to use the proxy. I highly recommend this method.

Google Drive / Google Apps @ Illinois

In addition, we will use Google Drive to share files. You should have an "infinite" amount of free storage on Google Drive, and you can set up Google Drive so that files are automatically synced to your computer. You may want to upload PDFs from the pre-lecture reading there; if you place these PDFs in the shared folder, please name them `FirstAuthorLastName-Journal-Year.pdf` so that they remain organized. The team slides will be made available using Google Apps.

This means that you will need to either:

- Use your personal Google account to access Google Apps. Be aware that this will count towards your Google storage limitations.
- Activate and use your campus Google account. See the FAQ and more information (including how to create your account).

Your campus Google account will be separate from an existing Google account, should you have one.

Lecture topics and reading calendar

Tuesday	Thursday	*notes*
1/21	1/23	introduction
1/28	1/30	Intro to materials science for nonexperts
2/4	2/6	Python for data science: Organizing data and Visualizing data ; filled in versions: organizing and scrubbing
2/11	2/13	
2/18	2/20	
2/25	2/27	Materials selection with Materials Project and Band Alignment slides, part 2 / Materials Project notebook Alignment Plot notebook / Data: descriptors, Data: density energy hull, Data: chemical compositions
3/4	3/6	Defect ID using statistical learning methods: Slides notebook
3/11	3/13	*no class* (APS meeting)
~~3/18~~	~~3/20~~	*no class* (spring break)

Tuesday	Thursday	*notes*
3/25	3/27	4CeeD Lecture 1; GaN Etch Experiment, 4CeeD: CreateAnAccount, 4CeeD Lecture1 Guide 2023 / 4CeeD LectureSeries ExtendedFeatures 2; 4CeeD Lecture2 Guide; 4CeeD JupyterDemo
4/3	4/5	4CeeD Lecture 3 (backend); 4CeeD Lecture 4 Slides, 4CeeD Lecture 4 Guide
4/8	4/10	Image processing for TEM: Paper; Handout, ImageJ; *Images*: RR_2143 STEM 4.6 Mx HAADF_25.1pA_1024px_2.0us_Raw_Stack_16bit: top right quarter, full image
4/15	4/17	Model development from first principles: notebook, notebook 2, slides, slides part 2
4/22	4/24	Graphene ResQ Neural network, Bayesian search, Gaussian process: Slides, Maruyama Matter paper; video and notebook
4/29	5/3	Graphene ResQ Neural network, Bayesian search, Gaussian process: notebook, slides
5/6	~~5/8~~	Uncertainty Quantification: slides, book chapter, notebook
5/13	5/15	*finals week*