MSE 598 -MATERIALS INFORMATICS

Instructor: J.C. Stinville, MSEB 201c, **jcstinv@illinois.edu**

TA: C. Bean, **cmbean2@illinois.edu**

Lecture: TR 12:30-1:50 pm, 2200 Sidney Lu Mech Engr (+lecture capture on MediaSpace)

Campuswire link: https://campuswire.com/p/G953DD6B2

Office hours: Request by email

MediaSpace Links:
https://mediaspace.illinois.edu/channel/MSE+598+JCS+2024+Spring/327694372

This course is essential for new learners and more experienced researchers. It covers:

1. The significance and unavoidable role of **materials informatics in your field**. You'll understand if and how the fundamental methods are relevant to your work.
2. Practical guidance on initiating and mastering specific algorithms. This includes adhering to the best practices in **data handling and software usage.**
3. Strategies for **integrating materials informatics** into your research and academic and professional journey.

4. Comprehension of **Experimental Techniques for Rapid Materials Characterization**

Recommended books:

- Krishna Rajan, Informatics for Materials Science and Engineering

Links to an external site., Butterworth-Heinemann, 2013, https://doi.org/10.1016/B978-0-12-394399-6.00021-7

- [Links to an external site.](https://www.sciencedirect.com/science/article/pii/B9780123943996000217).
  (https://www.sciencedirect.com/science/article/pii/B97801239439960
  00217)

Course Outline:

Applying machine learning (ML) to materials involves the following workflow:

- 1. **Data Collection**: Gathering a materials dataset, which can be computational or experimental, varying in size and source.
- 2. **Descriptors Identification:** Selecting effective features or descriptors for materials representation in ML, like composition vectors or elemental properties.
- 3. **Data Pre-Processing:** Standardizing, normalizing, and reducing dimensions of data before ML application.
- 4. **Learning Methods:** Choosing between supervised (finding patterns in labeled data) and unsupervised learning (finding patterns in unlabeled data).
- 5. **Algorithm Selection:** Selecting and testing different ML algorithms, like neural networks or random forest, based on data quality and descriptors.
- 6. **Data Splitting:** Dividing the dataset into training, validation, and testing sets for model optimization and accuracy testing.
- 7. **Hyperparameter Optimization:** Adjusting ML algorithm settings to enhance predictive performance.
- 8. **Application and Discovery:** Using ML models for new discoveries in materials science, such as predicting new materials properties or aiding in design and research.

The various class modules are structured to comprehensively outline this workflow:

- Introduction
- Materials Informatics (MI) and Data
- Data Visualization
- Machine Learning (ML)
- High-throughput measurements

Teaching approach:

- Teaching via reactive code notebooks: Reactive code notebooks like Jupyter and Pluto are popular web-based computing environments that allow

interactive coding, documentation, and multimedia inclusion such as images, plots, and videos. These notebooks are ideal for hands-on ML pratice.
- Demonstrating essential concepts using examples
- **Raising curiosity and confidence via competitions**

Grading:

- 30% 6 Reading\seminar assignments (keep 5 best scores)
- 40% 5 Homework
- 30% Term paper: on the topic of your choice, in groups of 3 students
- (+2% Attendance)

Thank you all for this great semester!

ACTIVE LEARNING APPROACH

- **Learning is an interactive process** - Ask and answer questions.
- **Come prepared to class** - Read and reflect on assigned reading in the textbook before lecture; prepare and post questions and answers on Canvas for reading assignments; use campuswire for other course-related questions. Read and study assigned articles and questions.
- **Participate actively during classes** - Share with the class your knowledge and interests in certain alloys and applications.

GRADING POLICIES

You are expected to have read the Student Code section related to Academic Integrity (http://admin.illinois.edu/policy/code/article1_part4_1-401.html). All infractions listed in the Student Code, including cheating and plagiarism, will result in penalties under the Student Code. If you have any questions regarding what constitutes an infraction, contact me.

HOMEWORK

There will be **five** homework assignments throughout the semester (roughly one every two weeks), each due on Friday by 5 pm. Late assignments will not be graded. You will complete these assignments through the Canvas website. Your overall assignment grade will be the average of your four best scores.

TERM PAPER/GROUP PRESENTATION

30% of the grade of this course will be based on a oral presentation and report, each group comprised of 3 students. You are free to choose your group members. The topic of your presentation should be specific and well defined, with a focus on materials informatics (ML approaches or High-throughput measurements) .

COVID

Following University policy, all students are required to engage in appropriate behavior to protect the health and safety of the community. Students are also required to follow the campus COVID-19 protocols. Students who feel ill must not come to class. In addition, students who test positive for COVID-19 or have had an exposure that requires testing and/or quarantine must not attend class. The University will provide information to the instructor, in a manner that complies with privacy laws, about students in these latter categories. These students are judged to have excused absences for the class period and should contact the instructor via email about making up the work.

Students who fail to abide by these rules will first be asked to comply; if they refuse, they will be required to leave the classroom immediately. If a student is asked to leave the classroom, the non-compliant student will be judged to have an unexcused absence and reported to the Office for Student Conflict Resolution for disciplinary action. Accumulation of non-compliance complaints against a student may result in dismissal from the University.

All students, faculty, staff, and visitors are required to wear face coverings in classrooms and university spaces. This is following CDC guidance and University policy and is expected in this class.

Please refer to the University of Illinois Urbana-Champaign's COVID-19 website for further information on face coverings. Thank you for respecting all of our well-being so we can learn and interact together productively.

To implement COVID-19-related guidelines and policies affecting university operations, instructional faculty members may ask students in the

classroom to show their Building Access Status in the Safer Illinois app or the Boarding Pass. Staff members may ask students in university offices to show their Building Access Status in the Safer Illinois app or the Boarding Pass. If the Building Access Status says "Granted," that means the individual is compliant with the university's COVID-19 policies—either with a university-approved COVID-19 vaccine or with the on-campus COVID-19 testing program for unvaccinated students.

Students are required to show only the Building Access Screen, which shows compliance without specifying whether it was through COVID-19 vaccination or regular on-campus testing. To protect personal health information, this screen does not say if a person is vaccinated or not. Students are not required to show anyone the screen that displays their vaccination status. No university official, including faculty members, may ask students why they are not vaccinated or any other questions seeking personal health information.

EMERGENCY RESPONSE RECOMMENDATIONS

Emergency response recommendations can be found at the following website: http://police.illinois.edu/emergency-preparedness/. I encourage you to review this website and the campus building floor plans website within the first ten days of class. http://police.illinois.edu/emergency-preparedness/building-emergency-action-plans/.

ANTI-RACISM AND INCLUSIVITY

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 for 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 many 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. The effectiveness of this course depends 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 Bias Assessment and Response Team (BART) (https://bart.illinois.edu/). Based on your report, BART members will follow up and reach out to students to ensure 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.

ADDITIONAL IMPORTANT TOPICS

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/resources/students/#confidential. Other information about resources and reporting is available here: wecare.illinois.edu.

Academic Integrity The University of Illinois at Urbana-Champaign Student Code should also be considered part of this syllabus. Students should pay particular attention to Article 1, Part 4: Academic Integrity. Read the Code at the following URL: http://studentcode.illinois.edu/. Academic dishonesty may result in a failing grade. Every student must review and abide by the Academic Integrity Policy: https://studentcode.illinois.edu/article1/part4/1-401/. Ignorance is not an excuse for any academic dishonesty. It is your responsibility to read this policy to avoid any misunderstanding. Do not hesitate to ask the instructor(s) if you are ever in doubt about what constitutes plagiarism, cheating, or any other breach of academic integrity.

Religious Observances Illinois law requires the University to reasonably accommodate its students' religious beliefs, observances, and practices regarding 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[https://odos.illinois.edu/community-of- care/resources/students/religious-observances/](https://odos.illinois.edu/community-of-care/resources/students/religious-observances/) to request appropriate accommodations. This should be done in the first two weeks of classes.

Disability-Related Accommodations To obtain disability-related academic adjustments and/or auxiliary aids, students with disabilities must contact the course instructor and the Disability Resources and Educational Services (DRES) as soon as possible. To contact DRES, you may visit 1207 S. Oak St., Champaign, call 333-4603, e- mail disability@illinois.edu or go to https://www.disability.illinois.edu. If you are concerned you have a disability-related condition that is impacting your academic progress; there are academic screening appointments available that can help diagnosis a previously undiagnosed disability. You may access these by visiting the DRES website and selecting "Request an Academic Screening" at the bottom of the page.

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 https://registrar.illinois.edu/academic-records/ferpa/ for more information on FERPA.

The course Syllabus outlines the essential content of the course and details what you need to know to be successful this year. As this course progresses, please refer to the syllabus when you need information about the course, such as 'How am I being graded?' and 'How do I contact my instructor?'.

Thank you.

I look forward to an excellent semester together!