THE UNIVERSITY OF WINNIPEG

APPLIED COMPUTER SCIENCE

Course Number: **GACS-7401-600**
Course Name: **Current Topics in Computing (Directed Readings):** Deep learning in Material Informatics

Instructor Information

Instructor: Qian Liu
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Meeting Time: Wednesdays/Fridays 10:30 - 12:00am 3D31

Important Dates

1.	First Class:	Wednesday, September 4, 2024
2.	Reading week (no classes):	October 13 – 19, 2024
3.	Last Class:	Wednesday, December 4, 2024
4.	Final Withdrawal Date w/o academic penalty*:	Wednesday, November 13, 2024
5.	University closures: Truth and Reconciliation Day	Monday, September 30, 2024
	Thanksgiving	Monday, October 14, 2024
	Remembrance Day	Monday, November 11, 2024

*A minimum of 20% of the work on which the final grade is based will be evaluated and available to the student before the voluntary withdrawal date.

Course Objectives / Learning Outcomes

Material informatics is an emerging interdisciplinary field that leverages data-driven approaches to accelerate the discovery, design, and deployment of new materials. Traditionally, materials science has relied heavily on experimental and theoretical methods to explore the vast space of possible materials and their properties. However, with the advent of deep learning, material informatics has gained a powerful tool to process and analyze large, complex datasets, enabling unprecedented insights and predictions.

Deep learning models, particularly neural networks, excel at recognizing patterns in data, making them well-suited for tasks such as predicting material properties, optimizing processes, and even discovering entirely new materials. These models can be trained on vast datasets of material compositions, structures, and properties, learning intricate relationships that might be difficult or impossible to capture with traditional methods.

One of the key advantages of deep learning in material informatics is its ability to generalize across different material systems, allowing researchers to make predictions about new materials with limited experimental data. This capability significantly reduces the time and cost associated with material development, paving the way for faster innovation in industries such as energy, electronics, and pharmaceuticals. As the field continues to evolve, deep learning is poised to become an integral part of material informatics, transforming how we approach materials research and development, and opening up new frontiers in the search for advanced materials.

Students enrolled in this course will explore the intersection of deep learning and material informatics. They will review and summarize key literature in the field, focusing on how deep learning techniques are applied to material discovery, characterization, and optimization. Throughout the course, students will also develop their scientific writing and oral presentation skills, with opportunities to contribute to research publications. By then end of the course, students will:

- Understand the Fundamentals of Material Science: Gain a comprehensive understanding of the principles underlying material science, including the structure-property relationships, crystallography, and thermodynamics that govern material behavior.
- Explore Advanced Characterization Techniques: Delve into the latest advancements in material characterization methods, such as X-ray diffraction (XRD), electron microscopy, and spectroscopy, and understand how these techniques are integrated with deep learning models to analyze and predict material properties.
- Grasp the Essentials of Materials Data and Databases: Learn about the vast array of materials data resources and databases, such as the Materials Project and AFLOW, and how these datasets are leveraged in deep learning models to accelerate material discovery and design.
- Investigate Multi-Modal Data Integration: Explore how deep learning enables the integration of multi-modal data sources, including experimental data, simulations, and theoretical calculations, to provide holistic insights into material properties and performance.
- Discover Machine Learning and Deep Learning Applications: Investigate the application of machine learning and deep learning techniques, including convolutional neural networks (CNNs), graph neural networks (GNNs), and reinforcement learning, in solving complex problems in material informatics.
- Develop Scientific Writing and Presentation Skills: Enhance scientific writing and oral presentation skills by reviewing, summarizing, and presenting findings from the literature in the field of material informatics and deep learning. Students will also have the opportunity to contribute to research papers and participate in discussions about emerging trends.

This course is designed to equip students with a thorough understanding of how deep learning is transforming material informatics. Through a multidisciplinary approach, students will learn to integrate material science principles with advanced computational techniques, preparing them for cutting-edge research and innovation in the field.

Evaluation Criteria

Weekly Progress Reports (20%)

- Participation: Students are required to attend weekly meetings to discuss their research progress.
- Written Report: A written report must be submitted to the instructor at least one day before each meeting. The report should include:
    - Completed Work: A summary of what was accomplished in the past week.
    - Upcoming Plans: A detailed plan for the following week.
    - Challenges: Any difficulties encountered, along with potential solutions.

Department Presentation (10%)

- Presentation: Students will prepare a 25-minute presentation on their research work, focusing on the application of deep learning in material informatics.
- Q&A Session: The presentation will be delivered to faculty members in the Department of Applied Computer Science, followed by a question-and-answer session where students must address faculty feedback and questions.

Final Report (65%)

- GOAL:
    - The final report should critically review the current state of research in material informatics, with a specific focus on the application of deep learning techniques. The report should explore how deep learning is being used to accelerate material discovery, analyze material properties, and integrate multi-modal data sources. It should also discuss the challenges and future directions of this interdisciplinary field.

- CONTENT:
    - Abstract (250 words maximum): Provide a concise summary of the report's scope, key findings from the literature, and major conclusions.
    - Introduction: Overview of material informatics and the role of deep learning in advancing this field. Introduction to the significance of integrating deep learning with traditional material science approaches.
    - Data Resources and Material Databases: Review key material databases such as the Materials Project and AFLOW, and discuss how they are utilized in deep learning applications.
    - Deep Learning Techniques in Material Informatics: Discuss various deep learning models (e.g., CNNs, GNNs) and their application in predicting material properties, optimizing processes, and discovering new materials.
    - Multi-Modal Data Integration: Analyze how deep learning integrates data from multiple sources, such as experimental data, simulations, and theoretical models, to provide comprehensive insights into material behavior.
    - Case Studies: Provide examples of successful applications of deep learning in material informatics, highlighting key findings and innovations.
    - Challenges and Future Directions: Discuss the challenges of applying deep learning in material informatics, including data quality, model interpretability,

and computational limitations. Explore potential future developments and research opportunities.
    - Conclusion: Summarize the main findings from the literature review and discuss the impact of deep learning on the future of material informatics.
    - Formatting Requirements:
        - Length: 20-30 pages, including references.
        - Figures and Tables: Appropriately labeled and referenced in the text.
        - Originality: Ensure the report is original, with all sources properly cited to avoid plagiarism.
        - Submission Deadline: TBD

- EVALUATION CRITERIA:
    - Students will be evaluated on the organization, content, depth of analysis, and overall presentation of the topics outlined in the Goal Section.

Students should contact the instructor as soon as possible if extenuating circumstances require missing a lab, assignment, test or examination. A medical certificate from a practicing physician may be required before any adjustments are considered.

Students with documented disabilities, temporary or chronic medical conditions, requiring academic accommodations for tests/exams (e.g., private space) or during lectures/laboratories (e.g., note-takers) are encouraged to contact Accessibility Services (AS) at 204-786-9771 or accessibilityservices@uwinnipeg.ca to discuss appropriate options. All information about a student's disability or medical condition remains confidential.
https://www.uwinnipeg.ca/accessibility-services.

Students may choose not to attend classes or write examinations on holy days of their religion, but they must notify their instructors at least two weeks in advance. Instructors will then provide opportunity for students to make up work examinations without penalty. A list of religious holidays can be found in the 2023-24 Undergraduate Academic Calendar online at http://uwinnipeg.ca/academics/calendar/docs/important-notes.pdf

Final Letter Grade Assignment

Historically, numerical percentages have been converted to letter grades using the following scale. However, instructors can deviate from these values based on pedagogical nuances of a particular class, and final grades are subject to approval by the Department Review Committee.

A+	90 – 100%	B+	75 – 79%	C	60 – 64%
A	85 – 89 %	B	70 – 74%	D	50 – 59%
A-	80 – 84%	C+	65 – 69%	F	below 50%

Required Text Book

There is no textbook for the course. The instructor will provide reading material in the form of journal papers, theses, and/or tutorials.

Prerequisite and Restriction Information

Consent of the Department Graduate Program Committee Chair or Instructor.

Regulations, Policies, and Academic Integrity

Students are encouraged to familiarize themselves with the Academic Regulations and Policies found in the University Academic Calendar at:
https://uwinnipeg.ca/academics/calendar/docs/regulationsandpolicies.pdf
Particular attention should be given to subsections 8 (Student Discipline), 9 (Senate Appeals) and 10 (Grade Appeals).

Avoiding Academic Misconduct: Academic dishonesty is a very serious offense and will be dealt in accordance with the University's policies.

Detailed information can be found at the following:

- Academic Misconduct Policy and Procedures: https://www.uwinnipeg.ca/institutional-analysis/docs/policies/academic-misconduct-policy.pdf and https://www.uwinnipeg.ca/institutional-analysis/docs/policies/academic-misconduct-procedures.pdf
- About Academic Integrity and Misconduct, Resources and FAQs: https://library.uwinnipeg.ca/use-the-library/help-with-research/academic-integrity.html

Uploading essays and other assignments to essay vendor or trader sites (filesharing sites that are known providers of essays for use by others who submit them to instructors as their own work) involves "aiding and abetting" plagiarism. Students who do this can be charged with Academic Misconduct.

Academic Integrity and AI Text-generating Tools: Students must follow principles of academic integrity (e.g., honesty, respect, fairness, and responsibility) in their use of material obtained through AI text-generating tools (e.g., ChatGPT, Bing, Notion AI). AI tools are permitted in this class. But students must cite them. According to the MLA (https://style.mla.org/citing-generative-ai/), writers should

- cite a generative AI tool whenever you paraphrase, quote, or incorporate into your own work any content (whether text, image, data, or other) that was created by it
- acknowledge all functional uses of the tool (like editing your prose or translating words) in a note, your text, or another suitable location
- take care to vet the secondary sources it cites

If students are not sure whether or not they can use AI tools, they should ask their professors.

Non-academic misconduct: Students are expected to conduct themselves in a respectful manner on campus and in the learning environment irrespective of platform being used. Behaviour, communication, or acts that are inconsistent with a number of UW policies could be considered "non-academic" misconduct. More detailed information can be found here:

- Respectful Working and Learning Environment Policy https://www.uwinnipeg.ca/respect/respect-policy.html,
- Acceptable Use of Information Technology Policy https://www.uwinnipeg.ca/institutional-analysis/docs/policies/acceptable-use-of-information-technology-policy.pdf
- Non-Academic Misconduct Policy and Procedures: https://www.uwinnipeg.ca/policies/docs/policies/student-non-academic-misconduct-policy.pdfand https://www.uwinnipeg.ca/policies/docs/procedures/student-non-academic-misconduct-procedures.pdf

Copyright and Intellectual Property: Course materials are the property of the instructor who developed them. Examples of such materials are course outlines, assignment descriptions, lecture notes, test questions, and presentation slides—irrespective of format. Students who upload these materials to filesharing sites, or in any other way share these materials with others outside the class without prior permission of the instructor/presenter, are in violation of copyright law and University policy. Students must also seek prior permission of the instructor/presenter before, for example, photographing, recording, or taking screenshots of slides, presentations, lectures, and notes on the board. Students found to be in violation of an instructor's intellectual property rights could face serious consequences pursuant to the Academic Misconduct or Non-Academic Misconduct Policy; such consequences could possibly involve legal sanction under the Copyright Policy:
https://copyright.uwinnipeg.ca/basics/copyright-policy.html

Privacy

Students have rights in relation of the collecting of personal data the University of Winnipeg

- Student Privacy: https://www.uwinnipeg.ca/privacy/admissions-privacy-notice.html
- Zoom Privacy: https://www.uwinnipeg.ca/privacy/zoom-privacy-notice.html

Class Cancellation, Correspondence with Students and Withdrawing from Course

When it is necessary to cancel a class due to exceptional circumstances, the course instructor will make every effort to inform students via uwinnipeg email and Nexus.

Students are reminded that they have a responsibility to regularly check their uwinnipeg e-mail addresses to ensure timely receipt of correspondence from the University and/or the course instructor**.**

Please let course instructor know if you plan on withdrawing from the course. Note that withdrawing before the VW date does not necessarily result in a fee refund.

Topics to be covered (tentative)

- Deep learning
- Machine learning
- Material informatics
- Multi-modal data integration

A permitted or necessary change in mode of delivery may require adjustments to important aspects of course outlines, like class schedule and the number, nature, and weighting of assignments and/or exams.