Materials Science in the Age of AI

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1 COURSE DESCRIPTION

This course examines the emerging intersection of AI and materials science, covering topics such as AI-driven materials discovery, property engineering, advanced characterisation, autonomous experimentation, data integration, sustainable materials, and real-time process optimisation. The course provides an "under-the-hood" view of how these models are built and run, equipping students with a deeper understanding of their mechanisms. By grasping how AI integrates into materials science, students will develop fresh conceptual approaches to tackling complex challenges in the field.

2 LEARNING OUTCOMES

- Gain a high-level understanding of key AI methodologies used in materials science and engineering, including machine learning, deep learning, computer vision, natural language processing, and autonomous research.

- Understand & implement the workings of commonly used AI/ML/DL algorithms and evaluation methodologies.

- Analyse & appreciate new technological developments in the field.

- Apply the latest methods and/or models to benchmarked materials datasets for meaningful statistical insights.

3 IMPLEMENTATION

Critial Analysis & Interpretation of Scientific literature :
How recent advances in mainstream AI models & key concepts have been borrowed and adapted into materials sciences.
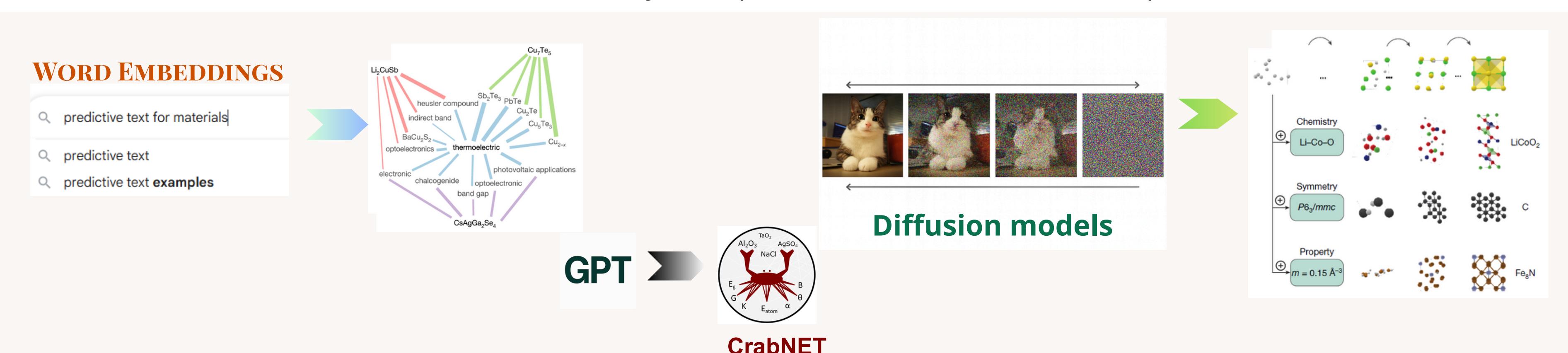
Explored ways in which GenAI tools can help/ hinder learning.

Student Feedback & Reflections

This course teaches the mindset and not only content. Very useful for practical applications Very encouraging on how to use AI to learn in a complementary way.

. Maybe I can make a flow chart by myself while reading the paper to help me better understand the main idea of the paper.

. Also I can read the paper with the help of other websites like the blog provided in this class to see what other people review on this paper.

Many examples are included in this course and I learn a lot about paper searching and reading skills.

Action Item

Ask ChatGPT (or ScSpace / Claude/Perplexity or any other multi modal AI that you may be familiar with)

You can upload the paper to the AI model, and ask it to summarize the paper.

Note that the quality of the answer will depend on your prompt.

Check if your idea of the paper aligns with that of the AI output.

You can keep the prompt and answer for later reference.

Sample Reflection

Question 3

Attempt this towards the end of the class: After We Discuss the paper in class
Reflecting on the learning you gained from analysing the paper:

Share your thoughts on your learning:

Do you think you learned more from analysing the paper?
What are the key insights / ideas or things that surprised you from the analysis?

In your own words please

4 REFLECTIONS & CHALLENGES

- Navigating abstract mathematical constructs and statistical concepts where students are predominantly from a non-mathematical or computer science background.
- Analysis of information dense literature requires a level of confidence in English which posed a challenge to a considerable number of students who are not native English speakers.
- the deeper mathematical and coding demands of this course made advanced model implementation difficult, despite code demonstrations provided in class.
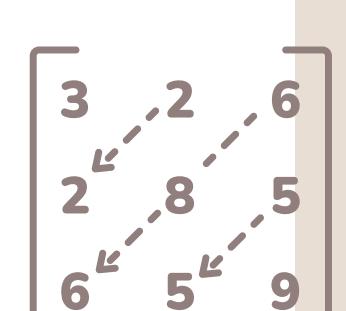
5 FUTURE

- Aim to develop interactive tools - such as visual notebooks or small coding modules that allow students to step through model computations in a hands-on, intuitive way to help bridge the gap between theory and practice, making abstract concepts more accessible and engaging.

Tshitoyan, V., Dagdelen, J., Weston, L. et al. Unsupervised word embeddings capture latent knowledge from materials science literature. Nature 571, 95–98 (2019).
Wang, A.YT., Kauwe, S.K., Murdock, R.J. et al. Compositionally restricted attention-based network for materials property predictions. npj Comput Mater 7, 77 (2021).
Zeni, C., Pinsler, R., Zügner, D. et al. A generative model for inorganic materials design. Nature 639, 624–632 (2025).