

### HOW MACHINE LEARNING IS REVOLUTIONISING MATERIALS SCIENCE PROFESSOR DANE MORGAN AND DR RYAN JACOBS

#### TO MAKE THE MOST OUT OF THIS SCRIPT, YOU COULD:

- Stick it in your book as a record of watching Dane and Ryan's animation
- Pause the animation and make notes as you go
- Add your own illustrations to the sheet
- Create your own animation to accompany it
- Add notes from classroom discussions
- Make notes of areas you will investigate further
- Make notes of key words and definitions
- Add questions you would like answered – you can message Dane and Ryan through the comments box at the bottom of their article:

**[www.futurumcareers.com/how-machine-learning-is-revolutionising-materials-science](http://www.futurumcareers.com/how-machine-learning-is-revolutionising-materials-science)**

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## SCRIPT:

Machine learning involves programming computers that 'learn' as they go. A part of artificial intelligence, machine learning looks for patterns in datasets and uses them to make decisions or predictions.

Professor Dane Morgan and Dr Ryan Jacobs, from the University of Wisconsin-Madison in the US, are investigating the opportunities and challenges posed by machine learning for the field of materials science and engineering (MS&E).

MS&E involves the study of materials' properties and the creation of new materials for specific purposes. Machine learning in MS&E is in its early stages but evolving rapidly.

Researchers in MS&E like Dane and Ryan now have access to massive digital databases that compile the structure and properties of countless materials. With powerful computing and modelling capabilities, it is becoming easier to explore and predict complex relationships between materials' structure, composition and their properties.

Most of this computing power comes from open-source software, with the fundamental machine learning algorithms available to everyone for free.

Machine learning is able to find patterns in huge datasets that would be impossible for humans to see. It can extract information from data to form links between a material's composition (the elements it contains) and structure (the position of atoms) to particular properties or functions.

For example, the brittleness of steel is affected by the type and distribution of atoms within its structure. Machine learning can be used to assess this, which is extremely useful for selecting a type of steel for a specific purpose – within a nuclear reactor, for instance.

As well as testing existing materials, ML can be used to predict structure-property-performance relationships in currently non-existent materials. Molecular-scale simulations are used to understand predicted properties as a key part of the discovery and design process.

For example, machine learning is being used to discover which materials can be used to make solar panels as efficiently as possible, by predicting how structural changes to a solar cell absorber material affect its ability to convert sunlight into electricity.

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Machine learning is also an effective means of data collection through natural language processing (NLP). Manually searching research papers for relevant information is massively time consuming, but NLP methods can extract information far more rapidly.

A lot of MS&E data is in the form of images. Researchers are often interested in finding individual objects in an image, such as missing atoms or defects.

Computer vision machine learning algorithms encode the complex relationships present in images – like contrast changes or the presence of edges around an object – enabling the algorithm to ‘learn’ what a particular microstructure or defect may look like.

Like all scientific fields, MS&E includes time-consuming tasks, such as mixing hundreds of combinations of different elements to test their properties. Increasingly, machine learning is performing these tasks, saving researchers a lot of time, effort and money.

Dane and Ryan believe that, in the future, each step of the scientific process, from hypothesis generation to running experiments to analysing results, will be aided by machine learning. This human-machine relationship will enable research to progress at an ever-increasing rate.

What would you investigate in the field of materials science and engineering?

How will you use machine learning in the future?

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