



University of
Sheffield

Centre for
Machine
Intelligence

**Registration for CMI AI Nibbles Seminar:
Materials Informatics for Alloy Discovery**

by [Prof. Nicola Morley](#)

Date: Thursday 9th May, 13:00 - 13:55

Location: Workroom 1, The Diamond

Abstract

The development of new alloys is critical for the realisation of novel technologies as well as instrumental in enabling improved performance. Complex concentrated alloys (CCAs), also often known as multi-principal element alloys or high entropy alloys, offer a promising avenue for alloy development, as their deviation away from a single base element opens up a vast compositional space that challenges traditional approaches, offering the possibility of significant material performance improvements from structural applications to advanced magnetics. However, this vast compositional space occupied by CCAs also poses a significant challenge, as efficient screening and downselection of promising compositions necessitates materials informatics tools, that in turn rely on the availability and robustness of large experimental databases that are currently scarce.

To this end, our work has focused on the development of an iterative approach utilising Machine Learning (ML) in a computational alloy downselection framework with an experimental high throughput make-test-characterise workflow to enable continual experimental database development, improve confidence in the computational framework predictions whilst also providing rapid material screening. In this talk our existing computational frameworks will be discussed (<https://doi.org/10.1063/9.0000657> and <https://doi.org/10.1002/adem.202302064>), outlining the materials informatics approaches used for constructing databases using natural language processing (NLP) and material discovery protocols using ML for both magnetics and structural metallics. Furthermore, our vision, in collaboration with the AIRE team will be detailed aiming to expand our activity across developing robust literature derived databases using large language models (LLMs) and NLP as well as further enhancing ML pipelines for materials discovery.

Please **enter your details below** to ensure you are added to the Google Calendar invite for this seminar:

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