



OPTiMA

ARC TRAINING CENTRE IN
OPTIMISATION TECHNOLOGIES
INTEGRATED METHODOLOGIES
AND APPLICATIONS

OPTiMA SEMINAR SERIES

MATERIALS INFORMATICS: ML-BASED OPTIMISATION FOR ACCELERATED MATERIALS ENGINEERING

The discovery of materials possessing a desired attribute is a holy grail of the materials engineering. "Forward design" – searching through parameter space to find favourable combinations that yield materials with some chosen characteristics – is commonly adopted. However, combinatorial space increases exponentially with dimensionality; therefore, such approaches can be hampered by the cost associated with exploration of vast swathes of parameter space as well as potential couplings between tunable parameters. With recent developments in machine learning (ML) algorithms and optimisation techniques, we now have a powerful arsenal to tackle issues associated with the common ad hoc trial-and-error forward design approaches.

Materials Informatics has emerged as a transformational discipline that integrates ML-based optimisation into the realm of materials design. Materials informatics enables development of novel "inverse design" methodologies, where a desired material property is explicitly targeted, and the parameters necessary to achieve it are found by a way of solving a constrained optimisation problem. Ellie is a computational soft matter physicist and engineer. The computational materials design tools that she has developed throughout her career are currently being used in chemical companies and government labs in US and Australia.

Following a two-year Fellowship at the University of Michigan, Ellie joined the Australian Defence Science and Technology Group (DSTG) in 2017 as a Research Scientist, where she established a research program in the field of Multiscale Simulation of Soft Matter and led a \$1.5 million Next Generation Technologies Fund project to develop an Integrated Multiscale Materials Simulation Platform for Advanced Acoustic Materials.

WED 1 DEC 4PM - 5PM AEST

ZOOM MEETING ID: 873 1557 5255; PASSWORD: 778635

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