

AI and ML in Materials Design and Discovery

NCI and Intersect Showcase

Four peak presentations will showcase state-of-the-art research activity aimed at speeding up materials design and discovery by integrating artificial intelligence (AI) and machine learning (ML) techniques.

Australian and international speakers reveal how large, high quality datasets coupled with machine learning analysis algorithms can play a vital role in the process of new material discovery.

The presentations will be of broad interest for scientists working into the field of HPC/Big Data in materials design and discovery, from advanced graduate research student level, to early career researchers and beyond.

13 May 2021

12pm - 4pm (AEST)

4am - 8am (CEST)

7pm - 11pm, 12 May (PDT)

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[Prof Kristin Persson \(UCB\)](#)

[Data-Driven Materials Innovation and Design: Examples from the Materials Project](#)



[Prof Shyue Ping Ong \(UCSD\)](#)

[Accelerating Materials Design through Automation and Machine Learning](#)



[Prof Amanda Barnard \(ANU\)](#)

[Classification, Correlation and Causation of Defects in Graphene Oxide Nanomaterials](#)



[Prof Nicola Marzari \(EPFL\)](#)

[The great acceleration in the design and discovery of novel materials](#)

Agenda:

12:00 – 12:05
12:05 – 12:55
12:55 – 13:00
13:00 – 13:50
13:50 – 13:55
14:00 – 14:50
14:50 – 14:55
15:00 – 15:50
15:50 – 16:00

Opening Remarks
Prof Kristin Persson
Question time
Prof Shyue Ping Ong
Question time
Prof Amanda Barnard
Question time
Prof Nicola Marzari
Question time

Chair:

[Prof. Michelle Spencer \(RMIT\)](#)

Co-organizers:

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