

# AI and ML in Materials Design and Discovery

## NCI and Intersect Showcase

Four peak presentations will showcase state-of-the-art research 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 materials discovery.

The presentations will be of broad interest for scientists working in 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:

11:55 – 12:00	Opening Remarks
<b>12:00 – 12:50</b>	<b>Prof Kristin Persson</b>
12:50 – 12:55	Question time
<b>13:00 – 13:50</b>	<b>Prof Shyue Ping Ong</b>
13:50 – 13:55	Question time
<b>14:00 – 14:50</b>	<b>Prof Amanda Barnard</b>
14:50 – 14:55	Question time
<b>15:00 – 15:50</b>	<b>Prof Nicola Marzari</b>
15:50 – 16:00	Question time

**Chair:** Prof Michelle Spencer (RMIT)

### Co-organizers:

Dr. Meiyun Chang-Smith  
(Graduate Education Program Manager, Intersect) Email: [meiyun@intersect.org.au](mailto:meiyun@intersect.org.au)

Dr. Jingbo Wang (Training Manager, NCI)  
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[For more information about the event, click here](#)