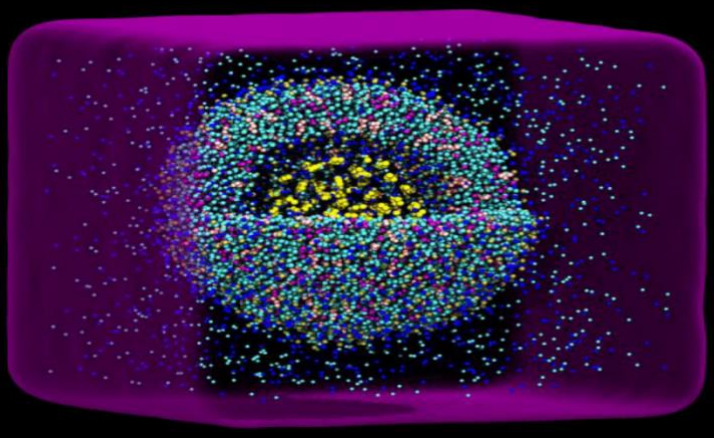
AI and ML in Drug Design and Discovery

Program



Presentation Timetable

26 May 2022	Prof Olexandr Isayev	Dr Arvind Ramanathan	Prof Cecilia Clementi	Prof Michele Vendruscolo
Canberra, Australia AEST Zone	**Pennsylvania, US EDT**	**Illinois, US CDT**	**Los Angeles, US PDT**	**Cambridge, UK BST**
12-1pm	10-11pm 25/5	9-10pm	7-8pm	3-4am
1-2pm	11-12am	10-11pm 25/5	8-9pm	4-5am
2-3pm	12-1am	11-12pm	9-10pm 25/5	5-6am
3-4pm	1-2am	12-1am	10-11am	6-7am 26/5

Agenda

11:50 - 12 noon **Zoom Webinar Open**

12 noon - 12:05 **Opening Remarks**



AEST 12:05 – 12:55

OLEXANDR ISAYEV

Accelerating Drug Discovery with Machine Learning and AI

ABSTRACT



AEST 13:00 – 13:55

ARVIND RAMANATHAN

A Supercomputing Perspective on AI-driven Drug Discovery for COVID-19

ABSTRACT



AEST 14:00 – 14:55

CECILIA CLEMENTI

Designing Molecular Models with Machine-Learning and Experimental Data

ABSTRACT



AEST 15:00 – 15:55

MICHELE VENDRUSCOLO

Towards the use of machine learning for drug discovery for protein misfolding diseases

ABSTRACT

AEST 16:00 – 16:05 **Closing Remarks**

(Image: *liposome* – Credit to A/Prof Defang Ouyang at Uni of Macau)