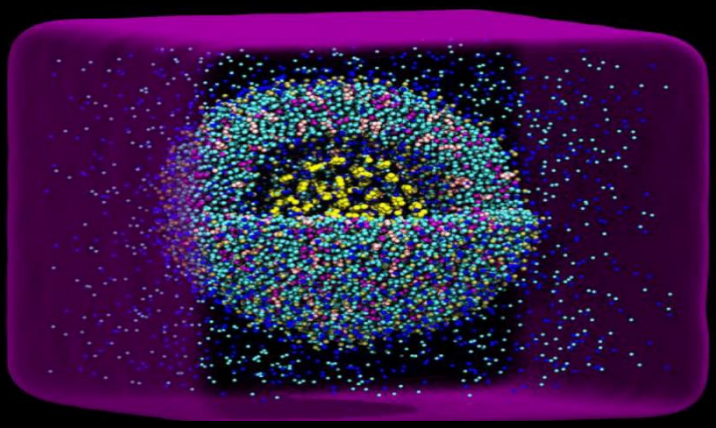
AI and ML in Drug Design and Discovery

Speakers





Designing Molecular Models with Machine-Learning and Experimental Data

ABSTRACT

Cecilia Clementi Cecilia Clementi is Einstein Professor of Physics at Freie Universität (FU) Berlin, Germany. She joined the faculty of FU in June 2020 after 19 years as a Professor of Chemistry at Rice University in Houston, Texas. Cecilia obtained her Ph.D. in Physics at SISSA and was a postdoctoral fellow at UC San Diego, where she was part of the La Jolla Interfaces in Science program. Her research focuses on the development and application of methods for the modelling of complex biophysical processes, by means of molecular dynamics, statistical mechanics, coarse-grained models, experimental data, and machine learning. Cecilia's research has been recognized by a National Science Foundation CAREER Award (2004), and the Robert A. Welch Foundation Norman Hackerman Award in Chemical Research (2009). Since 2016 she is also a co-Director of the National Science Foundation Molecular Sciences Software Institute.



Accelerating Drug Discovery with Machine Learning and AI

ABSTRACT

Olexandr Isayev is an Assistant Professor at the Department of Chemistry at Carnegie Mellon University. In 2008, Olexandr received his Ph.D. in computational chemistry. He was Postdoctoral Research Fellow at the Case Western Reserve University and a scientist at the government research lab. During 2016-2019 he was a faculty at UNC Eshelman School of Pharmacy, the University of North Carolina at Chapel Hill. Olexandr received the “Emerging Technology Award” from the American Chemical Society (ACS) and the GPU computing award from NVIDIA. The research in his lab focuses on connecting artificial intelligence with chemical sciences.



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

ABSTRACT

Arvind Ramanathan is a computational biologist in the Data Science and Learning Division at Argonne National Laboratory and a senior scientist at the University of Chicago Consortium for Advanced Science and Engineering (CASE). His research interests are at the intersection of artificial intelligence, high performance computing and biological/biomedical sciences. His research focuses on developing scalable AI methods for understanding complex biological phenomena including phase separation in biological systems as well as design of novel CRISPR/Cas9 probes to modify microbial functions. He obtained his PhD from Carnegie Mellon University and has been awarded the UT-Battelle Early Career Award (2017), apart from being recognized with the IEEE/ACM Gordon Bell Award for HPC in COVID-19 research (2019).



Towards the Use of Machine Learning for Drug Discovery for Protein Misfolding Diseases

ABSTRACT

Michele Vendruscolo is Professor of Biophysics, Director of the Chemistry of Health Laboratory and Co-Director of the Centre for Misfolding Diseases at the Department of Chemistry of the University of Cambridge, where he moved over 20 years ago. His work is aimed at establishing the fundamental principles of protein homeostasis and protein aggregation, and at exploiting these principles to develop methods for drug discovery in neurodegenerative diseases. He has published over 500 scientific papers and 20 patents and given over 500 invited lectures at international meetings.

Moderator



Ben Corry is Professor at the Research School of Biology at the Australian National University. He gained his PhD from the ANU in 2003, before holding successive ARC research fellowships at UWA. He returned to the ANU in a faculty position in 2012, where he held an ARC Future Fellowship. His research utilises molecular simulation to understand the structure and function of proteins as well as transport in synthetic systems, with applications in drug design and water treatment.

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