



THE UNIVERSITY of EDINBURGH

School of Engineering

IMP seminar

12:30-13:30 on **15th Aug 2023**

HBB_Classroom 4

Opportunity and challenge of artificial intelligence (AI) in drug delivery

Prof Defang Ouyang



ABSTRACT

In recent decades pharmaceuticals and drug delivery have become increasingly critical in the pharmaceutical industry due to longer time, higher cost, and less productivity of new molecular entities (NMEs). However, current formulation development still relies on traditional trial-and-error experiments, which are time-consuming, costly, and unpredictable.

With the exponential growth of computing capability and algorithms, in recent ten years, a new discipline named “computational pharmaceuticals” integrates with big data, artificial intelligence, and multi-scale modeling techniques into pharmaceuticals, which offered great potential to shift the paradigm of drug delivery. Computational pharmaceuticals can provide multi-scale lenses to pharmaceutical scientists, revealing physical, chemical, mathematical, and data-driven details ranging across pre-formulation studies, formulation screening, in vivo prediction in the human body, and precision medicine in the clinic. Several formulation cases in the area will be discussed, such as solid dispersion, microsphere and mRNA lipid nanoparticle.

SPEAKER

Prof. Ouyang has a multidisciplinary background in pharmaceuticals & computer modelling, with experience in academia and industry. He obtained his bachelor (2000) and master (2005) in pharmaceuticals from Shenyang Pharmaceutical University, China. He completed his PhD in pharmacy at The University of Queensland, Australia, in 2010 and progressed directly to his faculty position (Lecturer in Pharmaceutical, PI) at Aston University (UK). From the end of 2014, he moved to the University of Macau.

Since 2011, he has pioneered the integration of multi-scale modeling, artificial intelligence and big data techniques in the field of drug delivery – “computational pharmaceuticals”. He has published 2 books, 5 book chapters, over 80 refereed SCI journal papers, and over 100 invited talks. He held 11 approved patents, which had been used in medicinal products. He edited the first book <Computational Pharmaceutical - the application of molecular modeling in drug delivery> (John Wiley & Sons Inc., 2015) in this research area. He serves as the associate editor /editorial board of <Drug Delivery and Translational Research>, <Asian Journal of Pharmaceutical Sciences>, <Pharmaceutical Research>, <Pharmaceuticals> and <Journal of Pharmaceutical Sciences>. He is establishing the first global artificial intelligence (AI)-based formulation platform (FormulationAI). He successfully trained 6 PhD and 30 master students.