Department of Systems Engineering
香港城市大學
City University of Hong Kong

Artificial Intelligence-Driven Design and Synthesis of Drug Molecules

Artificial intelligence is increasingly becoming a transformative force in drug discovery and development, offering unprecedented opportunities to shorten development cycles, reduce R&D costs, and improve the success rate of candidate compounds. Drug molecular design is inherently a multi-objective optimization problem, requiring the simultaneous consideration and balancing of multiple factors, such as biological activity, toxicity, and pharmacokinetic properties. However, conventional computational approaches often face substantial challenges in addressing these complex and interdependent design objectives in an integrated manner. Furthermore, for newly proposed candidate molecules, ensuring the feasibility of their chemical synthesis remains a central bottleneck in translating molecular design into practical applications. In this talk, we will present our team's latest research progress in multi-objective molecular design and chemical reaction prediction, and further discuss future directions for AI-driven intelligent drug design systems.

28 April 2026 (Tue)

3:00 pm - 4:00 pm

YEUNG - P7303

Speaker

Dr. Yiping Liu

College of Computer Science and Electronic Engineering, Hunan University, China

Dr. Yiping Liu is a Professor in the College of Computer Science and Electronic Engineering at Hunan University. He received his Ph.D. in 2017 from the China University of Mining and Technology and Oklahoma State University. From 2018 to 2020, Dr. Liu worked as an Research Assistant Professor at Osaka Prefecture University (now Osaka Metropolitan University) in Japan. He joined Hunan University as an Associate Professor in 2020 and was promoted to Professor in 2025.

Dr. Liu's research focuses on AI4Science, multi-objective intelligent optimization, and drug discovery. He has published over 70 papers in leading journals and conferences. Additionally, he has led four national-level projects—including the NSFC Young Scientists Fund (Category B) [formerly the Excellent Young Scientists Fund] and two provincial-level projects.

All are welcome

Seminar 2025-2026, SYE14