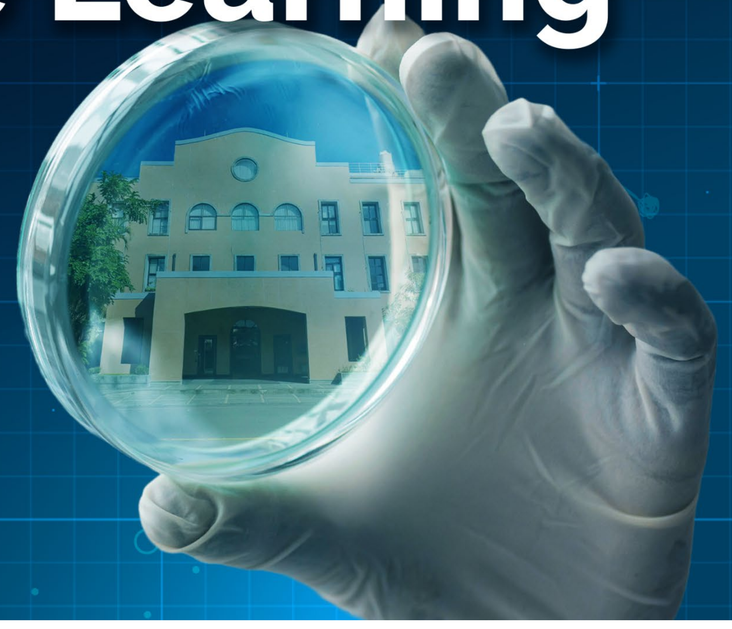
Chemistry Meets Machine Learning

June 15, 2023

Dr. Poe Lecture Hall,
Institute of Atomic and Molecular Sciences,
Academia Sinica



PROGRAM

08:30-09:20	REGISTRATION
09:20-09:30	**Opening: Prof. Hung-Wen Li (NTU)**
	Session Chair: Dr. Ching-Ming Wei (AS)
09:30-10:30	***Prof. William H. Green (MIT)*** *Quantitative Machine Learning for the Chemical Sciences*
10:30-10:45	Group Photo and Break
	Session Chair: Prof. Tzuhsiung Yang (NTHU)
10:45-11:30	**Prof. Yi-Pei Li (NTU)** *Introduction to Machine Learning: Exploring the Fundamentals and Applications*
11:30-12:30	**Prof. Yi-Pei Li and Mr. Shih-Cheng Li (NTU)** *Hands-on: Deep Learning for Molecular Property Predictions*
12:30-13:30	Lunch
	Session Chair: Prof. Ming-Kang Tsai (NTNU)
13:30-14:00	***Prof. Tzuhsiung Yang (NTHU)*** *Generative models for Chemistry: From ChatGPT to Molecular Design*
14:00-15:00	**Prof. Tzuhsiung Yang and Mr. Zhi-Hang Li (NTHU)** *Hands-on: A Demonstration of Inverse Design Using Ligands*
15:00-15:30	Q&A and Break
	Session Chair: Dr. Kaito Takahashi (AS)
15:30-15:40	**Dr. Pei-Kang Tsou (AS)** *"NN Potential Energy Surface"*
15:40-15:50	**Mr. Zong-Rong Ye (NTNU)** *"ML-way of Drug-Target Interaction"*
15:50-16:00	**Mr. Jia-Xian Yin (NYCU)** *"Our journey using Alphafold"*
16:00-16:15	**Dr. Mark Waller (Pending.AI)** *“Machine learning for Retrosynthesis”*
16:15-16:30	**Dr. Jurgen Swienty-Busch (Elsevier)** *“Reaxys Retrosynthesis in the hands of chemists”*
16:30-17:00	Q&A
17:00	Closing: Dr. Kaito Takahashi (AS)