

Solving Molecular Mysteries: How Computers and Artificial Intelligence are Changing the Way We Do Chemistry

破解分子之謎：電腦與人工智慧如何改變化學研究方式

Abstract 摘要

In this talk, we will step into the hidden world of molecules, the tiny building blocks that make up everything from medicines and plastics to the air we breathe. But here's the mystery: molecules are far too small to see, and their reactions can happen in a split second. So how do scientists figure out what's really going on? We will explore how computers help chemists "zoom in" on molecules, simulate their movements, and predict how reactions happen, almost like running a chemistry experiment inside a virtual laboratory. We will also examine how artificial intelligence (AI) is making this even faster and smarter, by learning patterns from huge amounts of chemical data and helping researchers discover new materials and new medicines. Along the way, you will learn how chemistry connects to real-life challenges like cleaner energy, better healthcare, and a more sustainable future and why the next generation of scientists might solve big problems with a mix of lab skills, computer power, and creative thinking.

在這場講座中，我們將走進分子的隱藏世界：這些微小的「積木」構成了我們身邊的一切，由藥物和塑料到我們呼吸的空氣。但這裏有一個謎團：分子小到肉眼無法看見，而它們的反應有時在一瞬間就發生。那麼，科學家究竟如何弄清楚其中真正發生了甚麼？我們將一起探索計算機如何幫助化學家「放大」分子世界，模擬分子的運動，並預測化學反應如何進行——幾乎就好像在虛擬實驗室裏做一場化學實驗。我們也會了解人工智能 (AI) 如何令一切變得更快、更聰明：它能夠從海量化學數據中學習規律，幫助研究人員發現新材料同新藥物。在這個過程中，你將看到化學如何與現實中的重大挑戰緊密相連，例如更清潔的能源、更先進的醫療，以及更加可持續的未來；也會明白為甚麼下一代科學家可能會把實驗技能、計算能力與創造力結合起來，去解決那些影響世界的大問題。

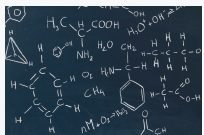
Speaker Biography 講者簡介

Prof. ZHANG Xinglong is the Assistant Professor in the Department of Chemistry at The Chinese University of Hong Kong. He received his BA in Natural Sciences from the University of Cambridge (2014), followed by an MSc in Theoretical and Computational Chemistry (2016) and a DPhil (2019) from the University of Oxford. After a postdoctoral stint at Caltech, he joined A*STAR, Singapore as a Research Scientist. His research focuses on computational catalysis (transition-metal-catalysed C-H functionalisation and asymmetric organocatalysis), workflow automation, and machine-learning methods for chemical discovery. He has published 50+ peer-reviewed papers in leading journals including *Nature*, *Nature Catalysis*, *Nature Synthesis* and *Nature Chemistry*.

章興龍教授現任香港中文大學化學系助理教授。他於2014年獲英國劍橋大學自然科學學士學位，隨後於2016年獲牛津大學理論與計算化學碩士學位，並於2019年獲博士學位。其後他在美國加州理工學院從事博士後研究，並加入新加坡 A*STAR 擔任研究科學家。他的研究聚焦於計算催化（過渡金屬催化的 C-H 官能團化與不對稱有機催化）、計算流程自動化，以及用於化學發現的機器學習方法開發與應用。他已在 *Nature*、*Nature Catalysis*、*Nature Synthesis* 與 *Nature Chemistry* 等頂尖期刊發表50餘篇同行評審論文。



Professor ZHANG Xinglong 章興龍教授
Department of Chemistry 化學系



Future Weather 未來天氣

Abstract 摘要

Has the weather in recent years become increasingly "abnormal"? Are extreme weather events becoming more frequent? Will future weather become unsuitable for human survival? In this lecture, we will explore together what changes scientists have discovered in the Earth's atmosphere in the past, how physicists and meteorologists use advanced technologies such as supercomputers, AI, satellites, and radar to forecast the future weather, and how the weather might become in the future in accordance with the latest research results. We will also demonstrate how to use simple instruments and physical principles to observe atmospheric conditions. We hope that this lecture will increase everyone's awareness of the climate crisis so that we can work together to protect the Earth's environment, which we depend on for survival.

近年的天氣是否越來越「不正常」？極端天氣是否越來越頻繁？未來的天氣會否變得不再適合人類生存？在這個講座中，我們將一起探討科學家發現地球大氣過去發生了什麼變化，物理學家及氣象學家怎樣利用超級電腦、AI、衛星、雷達等尖端科技預測未來天氣，而根據最新的研究，未來的天氣將會怎樣發展？我們亦會示範如何利用簡單的儀器和物理原理觀測大氣的狀況。期望是次講座能增進大家對氣候危機的覺察，同心協力，共同保護這個我們賴以生存的地球環境。

Speaker Biography 講者簡介

Professor LI Ping Wah is currently the Adjunct Assistant Professor in the Department of Physics at The Chinese University of Hong Kong. He was formerly a Senior Scientific Officer at the Hong Kong Observatory. Professor Li has long been engaged in research and services related to extreme weather forecasting and has considerable expertise in using computers and AI for weather prediction. He has also served as a team leader for a few working groups under the United Nations World Meteorological Organization's World Weather Research Programme, contributing to the advancement of forecasting technology and related services internationally.

李炳華教授現為香港中文大學物理系的客席助理教授，前為香港天文台高級科學主任。李教授長期從事極端天氣預報研究和服務，對利用電腦和AI預測天氣頗有心得。李教授亦曾擔任聯合國世界氣象組織世界天氣研究項目的小組主席，在國際間提高預報技術及相關服務。



Professor LI Ping Wah 李炳華教授
Department of Physics 物理系



香港中文大學理學院
FACULTY OF SCIENCE
THE CHINESE UNIVERSITY OF HONG KONG

The 20th Lau Oi Wah Memorial Science Lecture Series 第二十屆柳愛華紀念科學講座

Organized by The CUHK Faculty of Science and
The Lau Oi Wah Memorial Fund
香港中文大學理學院與柳愛華紀念基金主辦

17 April 2026 (Friday)
2:30 pm - 4:30 pm

LT4, Cheng Yu Tung Building (CYT), CUHK
香港中文大學鄭裕彤樓4號演講廳

鳴謝 Acknowledgements



Message from the Dean of Science

理學院院長的話



Welcome to the 20th Lau Oi Wah Memorial Science Lecture Series at The Chinese University of Hong Kong (CUHK). Commencing in 2005, this annual lecture series is organised in recognition of Professor Lau Oi Wah’s contributions to promoting science education.

Having obtained a BSc degree from The University of Hong Kong, Professor Lau joined Chung Chi College of CUHK as an Assistant Lecturer in 1968, whilst still working on her PhD thesis. She became a Lecturer at CUHK upon the completion of her doctoral studies in inorganic chemistry in 1970. After receiving the Leverhulme Foundation Fellowship in 1971 by Imperial College, London and the Honorary Research Fellowship in 1978 from the University of Birmingham, Professor Lau became a Chartered Chemist and an elected Fellow of the Royal Society of Chemistry, U.K., in 1981. Following her success in research in academia, Professor Lau was promoted to Senior Lecturer, in 1982, Reader in 1993, and was then elected to the Deanship of the Faculty of Science for three successive terms, from 1994 until her retirement in 2003.

Professor Lau was a devoted teacher and a caring research advisor, who always put her students’ learning and benefits first. During her academic career, she supervised seven PhD students and about 30 M.Phil. students. To those who knew her well, she was undoubtedly a passionate educator with a warm personality. During her Deanship, she successfully pushed for the establishment of many interdisciplinary teaching and research programmes, a philosophy of which continues to be a direction for curricula developments at the Faculty of Science. In addition to university teaching, Professor Lau had also initiated efforts to promotescience education in local secondary schools.

After the passing of Professor Lau, her friend and students established the “Memorial Fund of Professor Oi-wah Lau” in order to commemorate her commitment to eduction. Supported by the fund, the Lau Oi Wah Memorial Science Lecture Series runs annually to promote public engagement in science. The Lecture Series continues to inspire young people to pursue further studies and careers in scientific fields. Professor Lau’s legacy has indeed lived on through the gift of learning.

The Faculty of Science will continue to carry on Professor Lau’s legacy and devotion to promoting science to the general public. I hope today’s lectures will ignite your passion for science.

Chunshan SONG
Dean of Science
Wei Lun Professor of Chemistry

Programme Rundown

程序表

14:30

Opening Ceremony
開幕禮

14:40

Solving Molecular Mysteries:
How Computers and Artificial
Intelligence are Changing the Way
We Do Chemistry
破解分子之謎：電腦與人工智慧
如何改變化學研究方式

by Professor ZHANG Xinglong
Department of Chemistry
化學系 章興龍教授

15:30

Future Weather
未來天氣
by Professor LI Ping Wah
Department of Physics
物理系 李炳華教授

Biography of Professor Lau Oi Wah

柳愛華教授生平



The late Professor Lau Oi Wah devoted herself to promoting science education in both university and high school, and left a legacy of 35 years of service to The Chinese University of Hong Kong. As a Professor in the Department of Chemistry who also served as Dean of the Science Faculty from 1994 to 2003, Professor Lau Oi Wah recognised the importance of nurturing young minds of the next generation and the necessity to bringing scientific knowledge and advancement to the public.

Professor Lau joined the Department of Chemistry of Chung Chi College in 1968, and retired from the Faculty of Science of The Chinese University of Hong Kong in 2003. Active in affairs at both the college and university levels, Professor Lau served as Member of the University Council (1983–1986, 1994–2003), Member of College Assembly of Fellows (1980–2003), Member of College Board of Trustees (1986–1995), Chairperson of College Scholarships, Awards and Financial-Aid Committee (1977–1985), and Chairperson of College Physical Education Committee (1987–2003). During the nine years as the Dean of Science, Professor Lau led the Faculty of Science in building bridges between scientific frontiers and the masses, showing how science is an inherent as well as an integral part of everyday life. Even after retirement, Professor Lau continued to assist Chung Chi College in promoting campus health education.

After the passing of Professor Lau in 2004 at the age of 63, her former colleagues at the Faculty of Science wished to continue Professor Lau’s legacy in promoting science education to the young people of Hong Kong. First held in 2005, the annual Lau Oi Wah Memorial Science Lecture Series—jointly sponsored by the Faculty of Science and the Lau Oi Wah Memorial Fund—has been one of the ways the members of the Faculty of Science at The Chinese University of Hong Kong carry on Professor Lau’s dedication to igniting a passion for science among high school students.

柳愛華教授一生致力在大學及高中推廣科學教育，於中大春風化雨三十五載。柳教授一九六八年加入崇基學院化學系任教。二零零三年自中大榮休。在職期間，積極參與大學教務及書院服務。柳教授於一九九四至二零零三年間擔任理學院院長達九年，八三至八六年以及九四至零三年出任香港中文大學校董，於一九八零年至二零零三年參與崇基學院院務委員會工作，八六至九五年代表院務委員會出任崇基學院校董。一九七七年至一九八五年出任崇基學院獎學金委員會主席，又於一九八七年至二零零三年出任崇基學院體育委員會主席。柳教授於零三年榮休後，仍繼續匡助崇基學院的發展，出任學院資深導師，輔助推廣校園健康教育。

出任大學理學院院長九年間期，在柳教授的領導下，理學院擔任前線科學家及普羅市民的橋樑，與大眾一分享科研成果。柳教授致力培養年輕一輩學子對科學的熱情，以及將科學知識傳遞至各階層人士，拉近科學與香港市民的距離。

理學院全人非常認同柳教授在香港年輕人間群推動科學普及的理念，所以當柳教授在二零零四年辭世後，理學院也肩負起延續這份跟社會大眾傳達科學知識的責任。自二零零五年起，每年香港中文大學理學院與柳愛華紀念基金都會舉行「柳愛華教授紀念科學講座」，以延續柳教授獻身於推廣高中科普教育的無私精神。