

## PolyU Science Workshop

# AI x Science

**Date: 6 - 7 August 2025**

**Time: 09:00-17:30**

**Venue: Room Y301, 3/F, Lee Shau Kee Building (Block Y)**

**The Hong Kong Polytechnic University**

## PREFACE

The Faculty of Science is delighted to announce that the PolyU Science Workshop - AI x Science will be held on 6-7 August at PolyU. The two-day workshop aims to explore how artificial intelligence is revolutionizing the design, characterization, and modeling of advanced materials and functional devices. This interdisciplinary event will bring together materials scientists, computational researchers, and electrical engineers to examine the transformative potential of AI in accelerating innovation across semiconductors, energy storage, nanodevices, and smart materials.

The workshop will highlight cutting-edge applications of machine learning and data-driven approaches in materials science, devices, as well as computation models. Through keynote lectures and panel discussions, participants will explore how AI is overcoming traditional bottlenecks in materials research—from reducing trial-and-error experimentation to predicting emergent properties with unprecedented accuracy.

This workshop aims to foster partnerships between computational and experimental communities while addressing critical challenges in data quality, model transferability, and ethical AI deployment. We welcome you to join us to help shape the future of intelligent materials science and engineering, where data, algorithms, and domain expertise converge to redefine what's possible.

### Key Themes

- Generative models for novel materials
- AI-driven materials discovery  
(high-throughput screening, inverse design)
- Multiscale modelling  
(bridging quantum, atomistic, and continuum simulations)
- Smart characterization  
(automated microscopy, spectroscopy, and defect analysis)
- Device optimization  
(neural networks for photovoltaics, memristors, and sensors)

# Organizing Committee

## Chairman



### **Prof. Wai-Yeung WONG, Raymond**

Dean, Faculty of Science,  
Chair Professor of Chemical Technology,  
Department of Applied Biology and Chemical Technology,  
The Hong Kong Polytechnic University

## Co-Chairman



### **Prof. Yang CHAI**

Associate Dean (Research), Faculty of Science,  
Chair Professor of Semiconductor Physics,  
Department of Applied Physics,  
The Hong Kong Polytechnic University

## Members



### **Prof. Suting HAN**

Associate Professor,  
Department of Applied Biology and Chemical Technology,  
The Hong Kong Polytechnic University



### **Prof. Ming YANG**

Assistant Professor,  
Department of Applied Physics,  
The Hong Kong Polytechnic University

# Programme Rundown

## Day 1 | 6 August 2025 (Wednesday)

Start Time	Particular
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09:00-09:05	Welcome and Opening Address by <b>Prof. Wai-Yeung WONG, Raymond</b>
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### Session 1: AI for Science - Chaired by Prof. Yang CHAI

09:05-09:45	<b>Prof. Wanlin GUO</b> Nanjing University of Aeronautics & Astronautics <i>"Energizing Intelligence"</i>
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09:45-10:25	<b>Prof. Tiejun CUI</b> Southeast University <i>"AI for InfoMeta and InfoMeta for AI"</i>
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10:25-10:45	Coffee Break
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### Session 2: AI for Science - Chaired by Prof. Chaoliang TAN

10:45-11:15	<b>Prof. Qijie WANG</b> Nanyang Technological University <i>"Two-dimensional Mid-Infrared Sensor Enabling Simultaneous Perception and Encoding, and Hyperspectral Imaging"</i>
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11:15-11:45	<b>Prof. Shinhyun CHOI</b> Korea Advanced Institute of Science & Technology <i>"Development of Reliable Emerging Memory Devices and Future Perspectives"</i>
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11:45-12:15	<b>Prof. Wanyu LIN</b> The Hong Kong Polytechnic University <i>"Toward Interpretable Deep Learning for Molecular and Materials Science"</i>
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12:30-13:45	Lunch Break
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### Session 3: AI for Functional Materials – Chaired by Prof. Ming YANG

- 14:00-14:30    **Prof. Lianzhou WANG**  
The Hong Kong Polytechnic University  
*"Can Machine Learning Help Design Better Semiconductor Materials for Solar Energy Conversion?"*
- 14:30-15:00    **Prof. Jun YIN**  
The Hong Kong Polytechnic University  
*"Computational Insights into Degradation and Phase Segregation in Hybrid Perovskites using Machine Learning Potentials"*
- 15:00-15:30    **Prof. Wooyoung SHIM**  
Yonsei University  
*"Ion Transport within van der Waals Crystals"*
- 15:30-15:50    Coffee Break

### Session 4: AI for Functional Materials – Chaired by Prof. Zhong SUN

- 15:50-16:20    **Prof. Jizhou LI**  
The Chinese University of Hong Kong  
*"Computational Microscopy for Advanced Battery Characterization"*
- 16:20-16:50    **Prof. Ming YANG**  
The Hong Kong Polytechnic University  
*"A Physics-Informed Cluster Graph Neural Network Enables Generalizable and Interpretable Prediction for Material Discovery"*
- 16:50-17:20    **Prof. Quanhua MU**  
The Hong Kong Polytechnic University  
*"Decoding Cancer Evolution with Big Data and AI for Precision Medicine"*
- 17:20            End of Day 1

Day 2 | 7 August 2025 (Thursday)

Start Time	Particular
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Session 5: AI for Device Applications - Chaired by Prof. Qijie WANG

09:00-09:40	<b>Prof. Hongxia YANG</b> The Hong Kong Polytechnic University <i>"Co-GenAI: Exploring Collaborative Opportunities between Academic and Industry to Foster Innovation )"</i>
09:40-10:10	<b>Prof. Zhong SUN</b> Peking University <i>"Modern Analog Computing for Artificial Intelligence: Inference and Training"</i>
10:10-10:40	<b>Prof. Jing LI</b> The Hong Kong Polytechnic University <i>"From Words to Actions: The Pathway to NLP-Driven Embodied AI"</i>
10:40-11:00	Coffee Break

Session 6: AI for Device Applications - Chaired by Prof. Suting HAN

11:00-11:30	<b>Prof. Ran CHENG</b> The Hong Kong Polytechnic University <i>"EvoX: Evolutionary Computation as the Engine of Scientific Discovery"</i>
11:30-12:00	<b>Prof. Baile CHEN</b> ShanghaiTech University <i>"When III-V Photodiodes Meet AI: Enabling Miniaturized Spectrometers and Faster Optical Links"</i>
12:00-12:30	<b>Prof. Zongyin YANG</b> Zhejiang University <i>"Toward Next-Generation Spectral Detection: A Miniaturized High-Performance Solution"</i>
12:40-13:45	Lunch Break

### Session 7: AI for Science - Chaired by Prof. Tao WU

- 14:00-14:30    **Prof. Ni ZHAO**  
The Chinese University of Hong Kong  
*"Advancing Wearable Health Monitoring with Miniaturized Optoelectronics and Physiological Modeling"*
- 14:30-15:00    **Prof. Suting HAN**  
The Hong Kong Polytechnic University  
*"Self-powered Memristor for Biomimetic Sensory Computing"*
- 15:00-15:30    **Prof. Chaoliang TAN**  
City University of Hong Kong  
*"Two-Dimensional van der Waals Heterostructure-Based Memory Devices for Neuromorphic Computing"*
- 15:30-15:50    Coffee Break

### Session 8: Editor Sharing - Chaired by Prof. Lianzhou WANG

- 15:50-16:50    Editor Sharing
- **Dr Xin LI**, Springer Nature
  - **Dr Lu SHI**, Springer Nature
  - **Dr Yuen YIU**, Cell Press
- 16:50-16:55    Closing Remarks by **Prof. Yang CHAI**
- 16:55            End of Day 2





## Prof. Wanlin GUO

Chair Professor in Mechanics and Nanoscience

Institute of Nanoscience

Nanjing University of Aeronautics and Astronautics

**Prof. GUO** is the Academician of Chinese Academy of Sciences, and Chair Professor in mechanics and nanoscience at Nanjing University of Aeronautics and Astronautics. He received the National Science Foundation of China for Distinguished Young Scholars in 1996 and the honor of Cheung Kong Scholars in 1999. In 2012 and 2023, he obtained the National Nature Science Prize of China. He has published 600+ refereed papers in journals such as Science, Nature Nanotech, Nature Comm., Phys. Rev. Lett., Nano Lett., J. Am. Chem. Soc., Adv. Mater., J. Mech. Phys. Solids et al. His current research focuses on 1) three-dimensional fatigue fracture and damage tolerance and durability design of structures at high temperature; 2) intelligent nano materials and devices, multiscale physical mechanics, novel conception and technology for efficient energy conversion; 3) Hydrovoltaics and brain-like intelligence.

## Energizing Intelligence

Nature is always the best teacher for us to find better way to solve the problem. The intelligence of the living things is to survive by harvesting energy from the environment. Even the unicellular organism formed between 3.5 billion and 4.1 billion years ago in water can energize their intelligence through photosynthesis, metabolism and recently found hydrovoltaic effects. The currently widely applied artificial neuron network-based AI is inspired by the finding of neuron system in our brain more than one century ago. In sharp contrast to the energy hunger data center to support AI applications, we find that our brain can store huge information at  $10^{18}$  Bytes and process them at  $10^{18}$  floating point operations per second, equivalent to 78,000 latest generation Graphics Processing Units, but at the least energy consumption only 1.26 times of the theoretical limitation.

What is the scientific mechanism of the energy efficient biosystem and brain? What can we learn from it to create the next generation technology for neuron morphology computation in Memory? This talk will discuss these issues with the most cutting-edge advances.





## Prof. Tiejun CUI

Professor

Department of Electromagnetics and Microwave Technology  
Southeast University

**Prof. CUI** is the Academician of Chinese Academy of Science, IEEE Fellow, and Director of State Key Laboratory of Millimeter Waves, Southeast University. He proposed the concept of programmable metamaterials and established a new direction of information metamaterials, which bridge the physical world and digital world, and are easy to integrate with the artificial intelligence. He published over 700+ journal papers with more than 82000 citations (H-factor 137), and received many awards, including the National Natural Science Awards of China, Frontiers of Science Award in the First International Congress of Basic Science, IEEE ComSoc Marconi Prize, Tan Kah Kee Information Science Award, Leading Technology Award in World Internet Conference, and ACES Technical Achievement Award.

### AI for InfoMeta and InfoMeta for AI

In this presentation, I firstly introduce the concept and principles of information metamaterial (InfoMeta), and its relation with artificial intelligence (AI). Through digital coding representation, InfoMeta makes metamaterials be evolved from passive to active and from analog to digital and fuses the electromagnetic space and digital space. InfoMeta has three key features: 1) controls the electromagnetic waves in real time and in programmable way, fostering reconfigurable intelligent surface (RIS) technology and establishing a new paradigm for 6G intelligent programmable wireless environments; 2) controls the electromagnetic waves and processes digital information simultaneously, laying the foundation for electromagnetic information theory and developing new architecture for low-power wireless systems; and 3) is easy to integrate with AI technologies. I will present more details on how AI algorithms are used in InfoMeta to conduct intelligent and smart tasks, and how InfoMeta improves the AI technologies to build up intelligent systems and large electromagnetic models.



## Prof. Qijie WANG

President Chair Professor  
School of Electrical and Electronic Engineering &  
School of Physical and Mathematical Sciences  
Nanyang Technological University

**Prof. WANG** is a President Chair Professor at the School of Electrical and Electronic Engineering (EEE) and the School of Physical and Mathematical Sciences (SPMS) Nanyang Technological University. He is an OPTICA Fellow. He is a co-recipient of the Institution of Engineers Singapore, Prestigious Engineering Achievement Team Award of Singapore Twice in 2005 and 2017, respectively, the prestigious Singapore Young Scientist Award 2014, Nanyang Research Award 2015 (Young Investigator), ARC Sciences Nanotechnology Medal and Prize, 2021, and NTU College of Engineering Research Excellence Award, 2022.

### Two-dimensional Mid-Infrared Sensor Enabling Simultaneous Perception and Encoding, and Hyperspectral Imaging

It is becoming increasingly important to perceive, convert, and process a massive amount of data efficiently. However, the realization of these key functionalities, i.e. data perception, conversion, and processing, currently relies on a cascade of discrete modules including detectors, convertors, and processors, making the system bulky and inefficient. Here, assisted by machine learning, we present retina-inspired two-dimensional (2D) optoelectronic sensors based on 2D van der Waals (vdWs) heterostructure that can perform the data perception and conversion simultaneously, in the mid-infrared (MIR) regime, an important frequency band for night vision, sensing, spectroscopy, and free-space communications.



## Prof. Shinhyun CHOI

Associate Professor  
School of Electrical Engineering  
Korea Advanced Institute of Science and Technology

**Prof. CHOI** is KAIST Endowed Chair Professor and Associate Professor with tenure in the School of Electrical Engineering at Korea Advanced Institute of Science and Technology (KAIST). He graduated *Summa Cum Laude* from Seoul National University, Korea in 2009 with a Bachelor of Science in Electrical Engineering. He obtained his Master's and Ph.D. in Electrical Engineering at the University of Michigan, Ann Arbor in 2011 and 2015, respectively. He was a Postdoctoral Associate at Massachusetts Institute of Technology (MIT) from 2015 to 2018, where he investigated the fundamental understanding and neuromorphic applications of resistive switching devices. He has published his works in peer-reviewed articles including *Nature*, *Nature Materials*, *Nature Electronics*, *Nature Communications*, *Science Advances*, *Nano Letters*, *ACS Nano*. His works have been highlighted in *Nature News & Views*, *Nature Materials News & Views*, *Nature Electronics News & Views*, *Nature Nanotechnology Research Highlights*, *Nature Communications Editors' Highlights*.

## Development of Reliable Emerging Memory Devices and Future Perspectives

Artificial intelligence (AI) will enable machines to think and solve complex tasks like human beings. In recent years, artificial neural networks have improved recognition and classification accuracy. However, state-of-the-art deep learning algorithms require large network models with multiple layers, which pose significant challenges for complementary metal-oxide-semiconductor (CMOS) implementation due to limitations in conjoining computation, memory, and communication requirements in large networks. As an alternative hardware platform, emerging memories have been proposed for weight storage and fast parallel neural computing with low power consumption. The parallelism property of the crossbar arrays for matrix-vector multiplication enables significant acceleration of core neural computations. In this talk, Prof. Choi will present a systematic study on the fundamental understanding of emerging memory devices (RRAM and PRAM). He will talk about the approach how to achieve highly reliable artificial neurons and synapses for neuromorphic computing which can be a key step paving the way towards post von Neumann computing. In addition, he will also introduce the application of developed crossbar network, which suggests potential applications of emerging memory/computing device-based network to effective data processing for solving real-world problems. He will also talk about his recent work on phase change memory that shows low power consumption with cheap fabrication process.



## Prof. Wanyu LIN

Assistant Professor

Department of Computing &

Department of Data Science and Artificial Intelligence

The Hong Kong Polytechnic University

**Prof. LIN** is an Assistant Professor in the Department of Data Science and Artificial Intelligence and the Department of Computing at The Hong Kong Polytechnic University. She is serving as an Associate Editor for IEEE Transactions on Neural Networks and Learning Systems (TNNLS) and in Editorial Board of Memetic Computing. She is a member of ACM, IEEE. Prof. Lin's research focuses on developing trustworthy deep-learning techniques to accelerate scientific simulations and the design of molecular and materials science. She is the recipient of 2022 CVPR Best Paper Finalist and 2025 PolyU Young Innovative Researcher Award.

## Toward Interpretable Deep Learning for Molecular and Materials Science

Molecular and materials science lie at the heart of solving critical global challenges, from advancing healthcare and energy sustainability to driving environmental protection and next-generation technologies. Key application areas such as drug discovery, energy storage, carbon capture, catalyst development, and semiconductor innovation showcase the transformative potential of these fields. Central to these advancements is the intricate design and analysis of molecular and material systems, where traditional experimental and computational approaches are now being revolutionized by deep learning methodologies.

While deep learning excels in modeling complex chemical and physical phenomena, its "black-box" nature often hinders its ability to provide actionable scientific insights. This presentation focuses on the pivotal role of interpretability in deep learning. By fostering trust in predictions and enabling the extraction of meaningful mechanistic insights, interpretable frameworks empower scientists to uncover new principles and accelerate discovery systematically.



## Prof. Lianzhou WANG

Chair Professor of Global STEM

Department of Applied Biology and Chemical Technology

The Hong Kong Polytechnic University

**Prof. WANG** is a Chair Professor at Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University. Before moving to PolyU in June 2025, he has worked at The University of Queensland for over 20 years. His research focuses on the design and application of semiconductor nanomaterials for renewable energy conversion and storage including photocatalysts for solar fuel production, low-cost solar cells and rechargeable batteries. He has published > 600 articles in high quality journals including Science, Nature Energy, and Nature Nanotech, with a H-index of 132. He has won some prestigious honours/awards including Australian Research Council (ARC) QEII Fellowship (2006), Future Fellowship (2012), Laureate Fellowship (2019) and Industry Laureate Fellowship (2024), Scopus Young Researcher Award, and Research Excellence Award in Chemical Engineering of IChemE and RACI. He is elected fellow of the Australian Academy of Science (FAA), Australian Academy of Technological Sciences and Engineering (FTSE), and Academia Europaea (MAE), and is named on the Clarivate' Highly Cited Researchers list.

### Can Machine Learning Help Design Better Semiconductor Materials for Solar Energy Conversion?

Semiconductor nanomaterials hold the keys for solar energy conversion and storage systems like catalytic reactions for solar fuel production, low-cost solar cells, and rechargeable batteries. In this talk, we will give a brief overview of our recent progress in designing semiconductor nanomaterials for photoelectrochemical hydrogen generation and greenhouse gas conversion, low-cost solar cells with record-breaking efficiencies. Our journey in using machine learning to guide the selection of new dopants in semiconductor nanomaterials for photoelectrochemical water splitting showcases the potential of ML-powered material design strategy, which identifies the key parameters in dopant selection for transition metal oxide based photoelectrodes to achieve efficient charge separation and transport in water splitting reactions. The new findings could lead to new avenues for ML-guided material development towards renewable energy conversion and storage technologies.



## Prof. Jun YIN

Assistant Professor

Department of Applied Physics

The Hong Kong Polytechnic University

**Prof. YIN** is an Assistant Professor in the Department of Applied Physics at The Hong Kong Polytechnic University and holds the conferred title of Presidential Young Scholar. He has published over 240 research papers with h-index of 76, including publications in *Science*, *Nature*, *Nature Energy*, *Nature Photonics*, and *Nature Synthesis*. He is a recipient of the Excellent Young Scientists Fund from National Natural Science Foundation of China and has been recognized among the world's top 2% most-cited scientists by Stanford University from 2022 to 2024. His research focuses on leveraging machine learning to bridge theoretical insights with practical device applications, aiming to accelerate the development of next-generation materials for energy conversion and quantum technologies.

### Computational Insights into Degradation and Phase Segregation in Hybrid Perovskites using Machine Learning Potentials

I will present our recent advances in developing machine learning potentials (MLPs) for investigating hybrid perovskite materials, with a particular emphasis on how surface orientation and chemical composition influence surface and phase stability. By integrating MLP-enhanced molecular dynamics simulations, we achieve large-scale, long-timescale modeling of the FAPbI<sub>3</sub>/water interface. These simulations reconcile previously conflicting experimental observations and provide a quantitative basis for understanding the degradation mechanisms of hybrid perovskites. Additionally, we examine the structural heterogeneity arising from mixed A-site cation distributions in Cs<sub>0.5</sub>FA<sub>0.5</sub>PbI<sub>3</sub>. We introduce a new structural description (*i.e.*, heterogeneity coefficient) that captures the spatial distribution of cations. This descriptor effectively predicts organic cation rotation and octahedral distortion, both of which are critical to the electronic properties of heterogeneous perovskites. Our findings establish fundamental structure-stability relationships and offer a predictive framework to guide the rational design of more stable hybrid perovskite materials for next-generation photovoltaic applications.



## Prof. Wooyoung SHIM

Professor

Department of Materials Science and Engineering

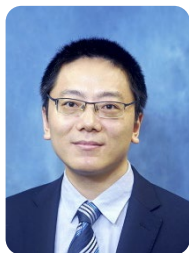
Yonsei University

**Prof. SHIM** is a Professor in the Department of Materials Science and Engineering at Yonsei University and Associate Dean of the College of Engineering. He received his Ph.D. from Northwestern University and completed postdoctoral research at Harvard University. He serves as Associate Editor of *Nano Letters* and Director of the Center for Multi-dimensional Materials. He is also an IBS Professor at the IBS Center for Nanomedicine. Prof. Shim has received several prestigious awards, including the President's Award from the National Research Foundation of Korea, the SKC Solmics Award, and the National Top 10 Nanotechnology Award.

### Ion Transport within van der Waals Crystals

The force–flux relationship provides a foundational framework for understanding mass transport under non-equilibrium conditions. Governed by the Onsager reciprocal relations, it captures how gradients in chemical potential—such as concentration, temperature, and electric potential—drive the transport of mass, heat, and charge, including their coupled cross-effects. In this presentation, I will discuss voltage-driven ion transport and its strong dependence on the characteristics of the diffusion medium. Particular emphasis will be placed on layered materials with van der Waals (vdW) gaps, which offer low energy barriers for ion migration. These vdW architectures present promising opportunities for applications across semiconductors, metals, and insulators, including their use in memory elements, switching devices, and ion-selective membranes.





## Prof. Jizhou LI

Vice-Chancellor Assistant Professor  
Department of Electronic Engineering  
The Chinese University of Hong Kong

**Prof. Li** is currently a Vice-Chancellor Assistant Professor in the Department of Electronic Engineering at The Chinese University of Hong Kong. With a background in mathematics and engineering, Prof. Li is dedicated to advancing transdisciplinary imaging science, fostering both methodological advancements and scientific discovery. His recent research focuses on computational X-ray microscopy for advanced battery characterization. Prof. Li has published over 50 peer-reviewed articles in prestigious journals and conferences, including *Science*, *Nature*, *Nature* research journals, *PNAS*, *Advanced Materials*, and *IEEE Transactions*. He has received several awards from IEEE and SIAM, and is a Senior Member of IEEE.

### Computational Microscopy for Advanced Battery Characterization

The rapid evolution of battery technologies is driving the demand for deeper and more precise characterization methods to unravel the complex mechanisms governing battery performance and degradation. X-ray microscopy has become an indispensable tool for non-destructive, high-resolution investigation of battery materials and architectures, enabling visualization of internal structures, interfaces, and dynamic processes during operation. However, conventional techniques face significant challenges in data reduction, analysis, and interpretation for specific tasks, requiring advanced computational methods to enhance their capabilities. In this talk, I will introduce our recent work on developing computational microscopy techniques and their applications in advanced battery material characterization. By creating synergy between X-ray microscopy, advanced computing, and scientific discovery, these advances could enable us to gain unprecedented insights into the evolution of materials within electrodes, ultimately driving technological innovation in battery materials science.



## Prof. Ming YANG

Assistant Professor

Department of Applied Physics

The Hong Kong Polytechnic University

**Prof. YANG** is currently an Assistant Professor in the Department of Applied Physics at The Hong Kong Polytechnic University (PolyU). He earned his Ph.D. from the National University of Singapore (NUS), where he also conducted postdoctoral research. Following this, Prof. Yang served as a Scientist at the Institute of Materials Research and Engineering in Singapore. Prof. Yang's research focuses on accelerating the development of functional materials for advanced applications through high-throughput screening, large-scale density first-principles calculations, and physics-informed machine learning. To date, Prof. Yang has authored or co-authored over 200 peer-reviewed articles in renowned journals, contributed to two book chapters, and filed three patents.

### **A Physics-Informed Cluster Graph Neural Network Enables Generalizable and Interpretable Prediction for Material Discovery**

Machine learning (ML) plays a pivotal role in the development of functional materials. However, achieving efficient, robust and interpretable predictions remains challenging due to the limited integration of domain knowledge. In this talk, I will introduce our proposed leveraging short-range atomic interactions of materials through a cluster graph representation to improve performance. This physics-informed cluster graph neural network (CG-NET) significantly enhances computational efficiency through a cluster sampling strategy. Importantly, by incorporating pseudo nodes as neighbors to the nodes at the cluster boundaries, we can maintain the coordination environment, ensuring prediction accuracy. I will further demonstrate CG-NET's remarkable prediction accuracy and efficiency across diverse material systems and properties and reveal its superior interpretability and generalizability with extensive experiments. Our work highlights the importance of integrating domain-specific scientific knowledge into the design of a generalizable and interpretable ML framework.



## Prof. Quanhua MU

Assistant Professor

Department of Applied Biology and Chemical Technology

The Hong Kong Polytechnic University

**Prof. MU** is an Assistant Professor in the Department of Applied Biology and Chemical Technology at the Hong Kong Polytechnic University. He received his bachelor and master's degree from Nankai University, and then completed PhD and postdoc training at The Hong Kong University of Science and Technology. He works on computational investigation of cancer evolution. Using bioinformatics and machine learning methods, his research has revealed multiple novel drug targets and drivers of drug resistance in brain cancer. His research has been published in journals such as *Cell*, *Science Translational Medicine*, *Nature Communications*.

### Decoding Cancer Evolution with Big Data and AI for Precision Medicine

Cancer remains the leading cause of human death. Recent developments have significantly improved patient prognosis, but the tumor cells keep evolving under treatment, leading to drug resistance and disease progression. Our prior work developed computational methods to track molecular evolution in brain tumors and uncovered novel therapeutic targets and resistance mechanisms. Recently, we focused on osteosarcoma, the most common primary bone cancer in children and adolescents. By integrating single-cell and multi-omics analyses, we characterized osteosarcoma's spatiotemporal heterogeneity, identifying four distinct cellular states linked to unique gene regulatory networks, tumor microenvironments, and treatment responses. To address data integration challenges, we developed scPoly, a single-cell foundation model that excels in batch effect correction and cell type annotation. Leveraging scPoly, we created OSpaedia.org, a comprehensive osteosarcoma data platform. These AI-driven innovations demonstrate the power of computational approaches in advancing biomedical discoveries and precision cancer medicine.



## Prof. Hongxia YANG

Associate Dean (Global Engagement)  
Faculty of Computer and Mathematical Sciences  
The Hong Kong Polytechnic University

**Prof. YANG**, PhD from Duke University, has published over 150 top conference and journal papers, and held more than 50 patents. She has been awarded the highest prize of the 2019 World Artificial Intelligence Conference, Super AI Leader (SAIL Award), the second prize of the 2020 National Science and Technology Progress Award, the first prize of Science and Technology Progress of the Chinese Institute of Electronics in 2021, the Forbes China Top 50 Women in Science and Technology and Ministry of Education Science and Technology Progress Award First Class in 2022 and AI 2000 Most Influential Scholar Award since 2023. She used to work as the ByteDance US LLM Head, AI Scientist and Director in Alibaba Group, Principal Data Scientist at Yahoo! Inc and Research Staff Member at IBM T.J. Watson Research Center. She founded the foundation model teams at both Alibaba and ByteDance and is a pioneer in the field of Generative AI.

## Collaborative Generative AI (Co-GenAI)

Generative AI (GenAI), including LLMs, MLLMs, and Stable Diffusion, is revolutionizing fields like healthcare, entertainment, and design. The market is projected to grow at 46.47% annually, reaching US\$356.1 billion by 2030. However, centralized GPU limitations hinder broad participation in model pretraining. To address this, we propose Co-GenAI—a decentralized, collaborative system that integrates hundreds of domain-specific models into a unified foundation model. Key innovations include: (1) Domain-Adaptive Continual Pretraining (DACP) for low-resource, domain-specific learning; (2) a scalable model-merging infrastructure leveraging high-quality inputs and ranking algorithms; and (3) an open platform for real-world deployment. This framework outperforms top models like Qwen2.5, LLaMA3.2, and Phi-4 across 11 benchmarks in reasoning, coding, and math, achieving ~10% average accuracy increment. Co-GenAI enables broader access, fosters inclusive development, and drives cross-disciplinary GenAI innovation.



## Prof. Zhong SUN

Assistant Professor  
Institute for Artificial Intelligence  
Peking University

**Prof. SUN** is a Boya Young Professor at Peking University, specializing in resistive random-access memory (RRAM) and emerging computing paradigms such as analog and in-memory computing. His research has been published in *PNAS*, *Nature Electronics*, *Nature Communications*, and *Science Advances*. His innovations have been consecutively adopted by the International Roadmap for Devices and Systems (IRDS) and recognized with the Intellectual Property Award (Italy, 2019), China's National High-Level Overseas Talents Program (2021), and the Intelligent Computing Innovators China award (2022). He serves the academic community as an Advisory Editorial Board Member for *APL Machine Learning*, Youth Editorial Board Member for *Chip*, and a regular reviewer for *Nature* journals and *PNAS*.

## Modern Analog Computing for Artificial Intelligence: Inference and Training

Modern analog computing with resistive memory (memristor) crossbars has emerged as an energy-efficient accelerator for neural network inference, mapping weights to conductances and performing parallel matrix-vector multiplications in a single time step. Building on this foundation, we extend analog computing to AI training. Closed-loop feedback circuits combining resistive memory crossbars with op-amps enable one-shot solutions to linear and least-squares systems, supporting on-chip matrix inversion, Fisher-information pre-conditioning, and other key operations for second-order optimization. A bit-sliced iterative refinement loop achieves full FP32 (24-bit fixed-point) accuracy for high-precision updates. To scale up, a block-matrix (BlockAMC) decomposition connects multiple sub-arrays without reprogramming, supporting large-model training. Measurements on foundry-fabricated 1T1R chips demonstrate up to 100× speed and energy improvements over GPUs at equal precision, paving the way for unified analog engines that integrate inference and training on the same resistive memory fabric.



## Prof. Jing Li

Associate Professor

Department of Computing

The Hong Kong Polytechnic University

**Prof. Li** is an Associate Professor and the Founder of the PolyU Embodied Artificial Intelligence Lab at PolyU-COMP. Previously, she served as an Assistant Professor at PolyU-COMP (2019–2025) and as a Senior Researcher at Tencent AI Lab (2017–2019). She earned her Ph.D. from CUHK in 2017 and her B.S. from Peking University in 2013. Prof. Li's research focuses on Natural Language Processing and Embodied AI. She has authored over 60 papers in top-tier venues. Her foundational model, AnglE, achieves millions of monthly downloads on Hugging Face and has been adopted by the U.S. unicorn Together.AI and the widely-used database MongoDB.

### From Words to Actions: The Pathway to NLP-Driven Embodied AI

Natural Language Processing (NLP) has evolved from addressing isolated tasks to building unified language representations, transforming how machines understand, generate, and reason about language and even knowledge. This talk highlights key milestones in NLP's evolution, with a focus on the rise of large language models (LLMs) and the state-of-the-art Retrieval-Augmented Generation (RAG) paradigm. We will explore the potential of LLMs as a cornerstone for Embodied Artificial Intelligence (Embodied AI)—systems that integrate perception, reasoning, and action seamlessly. While LLMs have begun to shape the early landscape of “thoughts,” they face significant challenges in grounding these capabilities in physical environments and translating knowledge into actionable behaviour. Looking ahead, this talk will discuss future directions for system-level NLP in Embodied AI, including multimodal integration, scalable deployment, and human-centred intelligence. By bridging the gap between words and actions, NLP is set to drive the next frontier of interactive and Embodied AI.



## Prof. Ran CHENG

Associate Professor

Department of Computing &

Department of Data Science and Artificial Intelligence

The Hong Kong Polytechnic University

**Prof. CHENG** is a jointly appointed Associate Professor (Presidential Young Scholar) in the Department of Data Science and Artificial Intelligence and the Department of Computing at The Hong Kong Polytechnic University. His research focuses on the evolvability of AI systems, aiming to develop multi-agent systems with autonomous learning and continual evolution capabilities for complex vertical applications. Prof. Cheng has published over 130 academic papers, with more than 17,000 citations on Google Scholar. His contributions have earned him several prestigious honors, including the IEEE Computational Intelligence Society Outstanding PhD Dissertation Award and the IEEE CIS Outstanding Early Career Award. He has been named a Clarivate Highly Cited Researcher for multiple consecutive years and is listed among the World's Top 2% Scientists by Stanford University. He serves as an Associate Editor for leading journals such as ACM TELO, IEEE TEVC, and IEEE TAI, and is the Founding Chair of the IEEE CIS Shenzhen Chapter.

## EvoX: Evolutionary Computation as the Engine of Scientific Discovery

As AI for Science advances, researchers are increasingly facing problems that lack explicit structure, exhibit black-box behavior, and offer little prior knowledge, thereby making them difficult to analyze, model, or optimize using conventional approaches. These challenges arise across a wide range of domains, from physics and engineering to biology and materials science. In this talk, I will introduce EvoX, an open-source platform built to support evolutionary algorithms—a family of population-based search methods inspired by natural evolution. Unlike traditional machine learning techniques that often require large datasets or clear gradients, evolutionary computation excels in exploring complex, non-differentiable, and data-scarce problem spaces, making it particularly suitable for many scientific applications. EvoX provides a high-performance computational backend that allows these algorithms to scale efficiently and be applied to large, high-dimensional design problems. I will showcase its application in supercritical airfoil design to illustrate how evolutionary approaches can enable intelligent search in domains where conventional methods often fail.





## Prof. Baile CHEN

Associate Professor  
School of Information Science and Technology  
ShanghaiTech University

**Prof. CHEN** is a tenured Associate Professor at the School of Information Science and Technology, ShanghaiTech University. His research focuses on advanced III-V photonic devices, such as ultra-high-speed uni-traveling-carrier (UTC) photodiode, high-speed mid-infrared photodetectors, miniaturized III-V semiconductor-based spectrometers. Prof. Chen has authored or co-authored 60 journal papers as first or corresponding author in prestigious journals, including *Nature Communications* and *Optica*. He currently serves as Associate Editor for *Optics Express* and is a Senior Member of IEEE.

### When III-V Photodiodes Meet AI: Enabling Miniaturized Spectrometers and Faster Optical Links

III-V semiconductor photodiodes serve as fundamental components for optoelectronic systems, with AI technologies now unlocking unprecedented performance. In this presentation, I will highlight two transformative applications of III-V photonics: (1) chip-scale single-pixel spectrometers enabled by our novel p-Graded-n architecture, offering compact, intelligent spectral analysis for portable sensing applications, and (2) record-breaking uni-traveling-carrier (UTC) photodiodes achieving >220 GHz bandwidth - a milestone that empowers next-generation AI optical interconnects with unprecedented data speeds. Together, these advancements demonstrate how the fusion of III-V photonics and AI is driving simultaneous breakthroughs in miniaturized spectroscopy and ultra-high-speed optical communications, opening new frontiers for smart sensing and computing systems.



## Prof. Zongyin YANG

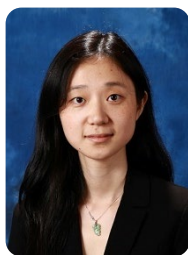
Qiushi Distinguished Professor  
College of Information Science and Electronic Engineering  
Zhejiang University

**Prof. YANG** is a Qiushi Distinguished Professor at Zhejiang University. He completed his B.S. in Mechanical Engineering and MSc in Optical Engineering at Zhejiang University. He was awarded his PhD in Electrical Engineering from the University of Cambridge in 2019, following which he served as a postdoctoral researcher and was selected as Research Fellow at King's College, University of Cambridge. Prof. Yang joined Zhejiang University as a Hundred-Talent Program Professor in 2020. He was selected as 'Innovators Under 35, China' by MIT Technology Review in 2021. He was selected as Alibaba DAMO Academy Young Scholars Award in 2023. He received Spark Award by HUAWEI in 2024. He got the high-level talent program (9 years) of National Science Fund in 2024. He became a tenured professor and was selected as the Qiushi distinguished professor of Zhejiang University in 2024.

Prof. Yang's research is focused on the miniaturization of optoelectronic devices. He has achieved significant breakthroughs, such as creating the world's smallest spectrometer and wavelength-tunable nanolaser. His research works have been published in top-tier journals, including *Science* (x2), *Nature Photonics*, *Science Advances*, *Nature Communications*, *Light S&A*, *Nano Letters*, and *JACS*, where he is the first/corresponding author.

### Toward Next-Generation Spectral Detection: A Miniaturized High-Performance Solution

This presentation highlights the groundbreaking development of miniaturized, high-performance spectrometers driven by advanced computational strategies. We present a series of breakthroughs from our research group, including the world's smallest spectrometer, the world's most efficient spectrometer, and the world's cheapest spectrometer. We will discuss how these novel devices are being deployed in critical real-world applications such as defect inspection in solar power plants, non-invasive glucose monitoring, and light source detection in optical communication systems. The talk will conclude with future perspectives on AI-driven spectral sensing and its transformative potential across scientific and industrial domains.



## Prof. Ni ZHAO

Professor

Department of Electronic Engineering

The Chinese University of Hong Kong

**Prof. ZHAO** is a Professor in the Department of Electronic Engineering at The Chinese University of Hong Kong. She received her Bachelor's degree from Tsinghua University in 2002, a Master's degree from McMaster University in 2004, and a Ph.D. from the University of Cambridge in 2008. Following her doctoral studies, she conducted postdoctoral research at the Massachusetts Institute of Technology from 2008 to 2010. She joined The Chinese University of Hong Kong in 2010 and currently holds the position of Full Professor. Prof. Zhao's research focuses on optoelectronic devices and wearable sensors for biomedical applications. Her work has resulted in over 190 publications in leading journals, with an h-index of 76, and has earned her multiple accolades, including recognition as a Highly Cited Researcher by Clarivate Analytics in 2018 and RGC Senior Research Fellow in 2024. Prof. Zhao is a Fellow of the Royal Society of Chemistry and a member of The Hong Kong Young Academy of Sciences. She also serves as Associate Editor for Science Advances.

### Advancing Wearable Health Monitoring with Miniaturized Optoelectronics and Physiological Modelling

The integration of advanced optoelectronic devices into wearable and contactless health monitoring systems is revolutionizing remote healthcare, particularly for aging populations managing chronic conditions like cardiovascular diseases. This talk highlights the development of a micro-sized optical spectrometer based on photomultiplication-type organic photodetectors, capable of bias-tunable spectral response and computational light reconstruction. With a footprint of just  $0.0004 \text{ cm}^2$  and sub-5-nm resolution, this spectrometer eliminates the need for bulky optics, offering unparalleled miniaturization, scalability, and cost-efficiency for sensor arrays in wearable diagnostics. In the second part, I will introduce physiological models that transform sensor outputs into actionable health data. Notably, the multi-wavelength photoplethysmography (PPG) technology sets a benchmark for cuffless blood pressure monitoring. Complementing this, the systemic reflection coefficient model translates optical data into cardiovascular parameters, enabling comprehensive disease assessment. Together, these innovations promise to redefine non-invasive, real-time health monitoring.



## Prof. Suting HAN

Associate Professor

Department of Applied Biology and Chemical Technology

The Hong Kong Polytechnic University

**Prof. HAN** is an Associate Professor in the Department of Applied Biology and Chemical Technology at The Hong Kong Polytechnic University. She received Ph.D. in Physics and Materials Science from City University of Hong Kong, Hong Kong SAR in 2014. From 2014 to 2016, she was a Postdoctoral Research Fellow at City University of Hong Kong. She joined Shenzhen University in 2016 as Associate Professor (tenure track) and was promoted to Full Professor (tenured) in 2021 and then Distinguished Professor in 2022. She was Visiting Professor in Department of Electrical Engineering and Computer Science at the University of Michigan, US in 2019. She joined The Hong Kong Polytechnic University as Associate Professor (tenured) in 2023. Her research interest includes flash memory, memristor, neuromorphic computing and in-memory computing systems. To date Prof. Han has published over 160 journal articles with 15,000 citations and h-index of 67 (Google Scholar) as first and corresponding author. She is the reviewer for over 50 journal including *Science*, *Nature* etc. Prof. Han is an Associate Editor of *Journal of Materials Chemistry C* and *Materials Advances*. She is an awardee of NSFC Excellent Young Scientist Fund and she has been listed as world's top 2% scientists by Stanford University (career-long impact).

### Self-powered Memristor for Biomimetic Sensory Computing

Anemotaxis behaviors inspired by rats have tremendous potential in efficiently processing perilous search and rescue operations in the physical world, but there is still lack of hardware components that can efficiently sense, encode, and recognize wind signal. Here, we report an artificial vibrissal system consisting of a self-powered carbon black sensor and threshold-switching HfO<sub>2</sub> memristor. By integrating a forming HfO<sub>2</sub> memristor with a self-powered angle-detecting hydro-voltaic sensor, the spiking sensory neuron can synchronously perceive and encode wind, humidity, and temperature signals into spikes with different frequencies. Furthermore, to validate the self-powered artificial vibrissal system with anemotaxis behavior, a robotic car with equipped artificial vibrissal system tracks trajectory toward the air source has been demonstrated. This design not only addresses the high energy consumption and low computing issues of traditional sensory system but also introduces the multimode functionalities, therefore promoting the construction of neuromorphic perception systems for neurorobotics.



## Prof. Chaoliang TAN

Associate Professor

Department of Electrical Engineering &

Department of Biomedical Engineering

City University of Hong Kong

**Prof. TAN** is currently an Associate Professor in the Department of Electrical Engineering and Department of Biomedical Engineering at the City University of Hong Kong. He received his PhD from Nanyang Technological University in 2016. After working as a Research Fellow in the same group for about one year, he then worked as a Postdoctoral Researcher at the University of California, Berkeley, for two years. His research focuses on 2D materials for electronics and optoelectronics, and structural engineering of layered materials for biomedicine, energy storage, etc.

### Two-Dimensional van der Waals Heterostructure-Based Memory Devices for Neuromorphic Computing

This presentation introduces advancements in neuromorphic computing enabled by van der Waals (vdW) heterostructures. The research team, led by the PI, has leveraged the superior electronic and optoelectronic properties of Te/Se to design and fabricate a variety of advanced memory devices. These include electronic/optoelectronic memory devices using a Te/h-BN/Gr/CIPS vdW heterostructure, floating-gate memory devices with a MoS<sub>2</sub>/h-BN/Te vdW heterostructure, and photoinduced memory devices featuring a MoS<sub>2</sub>/h-BN/Se vdW heterostructure. These devices are designed for neuromorphic computing applications, such as reservoir computing at the optical communication band, multimodal reservoir computing, and in-sensor compressing. Additionally, the team has also explored a range of engineering techniques, such as phase and defect engineering, to facilitate the fabrication of advanced flash memory devices using a MoS<sub>2</sub>/h-BN/1T'-MoTe<sub>2</sub> heterostructure, and reconfigurable memory devices with a MoS<sub>2</sub>/CIPS heterostructure for multifunctional neuromorphic computing tasks. This promising progress underscores the opportunities of vdW heterostructure-based multifunctional memory devices in advancing neuromorphic computing.



## Dr Xin Li

Senior Editor  
Springer Nature

**Dr Li** received her first degree in materials science and engineering from Shanghai Jiao Tong University in China. She completed her Ph.D. jointly at Georgia Institute of Technology and University of Lorraine, studying epitaxy growth and optoelectronic applications of wide bandgap semiconductors. She continued to work in the Georgia Tech-CNRS UMI as a postdoctoral researcher, and expanded her interests to 2D materials, nanostructures and flexible devices. At Nature Materials, which she joined in April 2017, Dr Li handles manuscripts in the areas of structural materials, nanomaterials synthesis, and 2D electronics. Dr Li is based in the Shanghai office.



## Dr Lu Shi

Senior Editor  
Springer Nature

**Dr Shi** joined Nature Nanotechnology as an editor in April 2023, bringing extensive experience from her previous roles as Editor-in-Chief of *Advanced Electronic Materials* and Deputy Editor of *Advanced Materials* at Wiley. Before embarking on her editorial career, Dr Shi's research focused on 2D materials growth and the magnetoelectric transport behavior of van der Waals heterostructures. She received a joint Ph.D. in Materials Science and Physics from the Université Catholique de Louvain, Belgium, and Université Grenoble Alpes, France. She covers a broad range of topics across electronics and optoelectronics in the journal.



## Dr Yuen YIU

Senior Editor  
Cell Press

**Dr YIU** obtained his PhD in condensed matter physics from the University of Tennessee and Oak Ridge National Laboratory, and did postdoctoral research at Ames Laboratory. Before joining Cell Press, he had worked as a popular science reporter and editor at the American Institute of Physics, and at *Science* as a commissioning editor. At *Device*, he alongside the editorial team oversees a wide scope of articles ranging from implantable biomedical devices to virtual reality displays. He is fluent in English, Mandarin, and Cantonese. He is currently based in Hong Kong.









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