Thu. Sep 3, 2026

Keynote

10:25 AM - 11:05 AM JST | 1:25 AM - 2:05 AM UTC | Hall A(International Confererence hall)

Plenary Talk

Chairperson: Hideaki Hisamoto

10:25 AM - 11:05 AM JST | 1:25 AM - 2:05 AM UTC

[Plenary Talk] **Infrared spectral pathology. Are we closer to clinical adoption?**

Peter Gardner (University of Manchester)

Keynote

2:50 PM - 3:30 PM JST | 5:50 AM - 6:30 AM UTC | Hall A(International Confererence hall)

Plenary Talk

Chairperson: Hideaki Hisamoto

2:50 PM - 3:30 PM JST | 5:50 AM - 6:30 AM UTC

[3XYIat90] **Droplet confined colloidal assembly and applications**

Lingling Shui (South China Normal University)

Keynote

3:30 PM - 4:10 PM JST | 6:30 AM - 7:10 AM UTC | Hall A(International Confererence hall)

Plenary Talk

Chairperson: Kiichi Sato

3:30 PM - 4:10 PM JST | 6:30 AM - 7:10 AM UTC

[9budaVfT] **MOF Crystallography of Microgram-Scale Bioactive Molecules**

Masaki Kawano (Institute of Science Tokyo)

Fri. Sep 4, 2026

Keynote

10:15 AM - 10:55 AM JST | 1:15 AM - 1:55 AM UTC | Hall A(International Confererence hall)

Plenary Talk

Chairperson: Deniel Citterio

[Plenary Talk] **From data accquisiton to knowledge generation: The trandformative role of artifical intelligence in analytical chemistry**

Pai-Shan Chen (National Taiwan University)

Keynote

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[Plenary Talk] **Computational and machine learning approaches for the identification of unknown chemicals by mass spectrometry**

Han Bin Ph (Sogang University)

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[Plenary Talk] **Infrared spectral pathology. Are we closer to clinical adoption?**

Peter Gardner (University of Manchester)

Infrared spectral pathology. Are we closer to clinical adoption?

Dougal Ferguson[1,2], Ashwin Sachdeva[3,4], Peter Gardner[1,2]

[1]Department of Chemical Engineering, and [2]Photon Science Institute University of Manchester, Oxford Road, Manchester, UK, University of Manchester, Oxford Road, Manchester, UK
[3]Division of Cancer Sciences, University of Manchester, UK
[4]Department of Surgery, The Christie Hospital NHS Foundation Trust, UK

Biographical Sketch

Peter Gardner is a Professor of Analytical and Biomedical Spectroscopy in the Department of Chemical Engineering and the Photon Science Institute at the University of Manchester. He obtained his BSc in Chemistry from the University of East Anglia in 1984 and his PhD in 1988. This was followed by post-doctoral positions at the Max Planck Institute in Berlin and the University of Cambridge. He is a physical chemist with 40 years of research experience in the field of infrared and Raman spectroscopy. In 1999 he turned his attention to applying infrared microscopy to the analysis of cells and tissue. He has been developing new methods to analyse tissue samples from biopsies with a view to helping pathologists better diagnose cancer. In particular he has been an early adopter of quantum cascade laser (QCL) based imaging which is poised to revolutionise spectral pathology. He is currently president of the international society for clinical spectroscopy CLIRSPEC

Abstract

The coupling of focal plane array detectors with infrared microscopes ushered in a new age of infrared hyperspectral imaging and stimulated the field of infrared spectral pathology. Numerous papers have been published demonstrating that the spectra contain key chemical information regarding disease state. Tissue classification using machine learning can be achieved with high degrees of accuracy meaning that the technique is potentially ripe for clinical adoption. Frustratingly, however, despite years of continued effort the field has hardly progressed beyond the proof-of-concept stage. This has been due to a number of factors. Firstly, FTIR imaging instruments are still too slow for a busy pathology lab, taking many hours to image a single piece of tissue. Secondly, the emergency of digital pathology means that tissue classification tasks can often be done based on a standard H&E image with no additional equipment. Thirdly we have been trying to replicate pathology and reduce the subjectivity of the assessment rather than helping clinicians to make treatment decisions. In this presentation I will explain how we have tackled all three of these problems using Quantum Cascade Laser based IR imaging[1], advanced deep learning[2] and predicting outcome data rather than tissue classification[3].

1. Dougal Ferguson, Niels Kroeger-Lui, Domenic Dreisbach, Claire Hart, Diego Sanchez, Pedro Oliveira, Mick Brown, Noel Clarke, Ashwin Sachdeva, and Peter Gardner, “Full fingerprint hyperspectral imaging of prostate cancer cohorts within clinical timeframes using novel quantum cascade laser microscopy”, *Analyst*, *150***,** 1741-1753, (2025).

2. Lyra OLeary; Dougal Ferguson; Claire Hart; Mick Brown; Pedro Oliveira; Noel Clarke; Ashwin Sachdeva; Peter Gardner; Hujun Yin , “Spatial-Spectral Deep Learning for Prostate Cancer Tissue Classification in Infrared Spectroscopy”, *Analytical Chemistry*. *98 (4)*, 2743-2755 (2026).

3. Dougal Ferguson, Ashwin Sachdeva, Claire A. Hart, Diego F. Sanchez, Pedro Oliveira, Mick, Brown, Noel Clarke, Peter Gardner, “Identification of at-risk prostate cancer patients using Fourier transform infrared spectroscopy and machine learning”, Proceedings Volume 13311, Optical Biopsy XXIII: Toward Real-Time Spectroscopic Imaging and Diagnosis; 1331103 (2025)

Keynote

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Plenary Talk

Chairperson: Hideaki Hisamoto

2:50 PM - 3:30 PM JST | 5:50 AM - 6:30 AM UTC

[3XYIat90] **Droplet confined colloidal assembly and applications**

Lingling Shui (South China Normal University)

Droplet Confined Colloidal Assembly and Applications

Lingling Shui
South China Normal University, Guangzhou 510006, P. R. China

Biographical Sketch

Dr. Lingling SHUI received the B.Sc. and M.Sc. degrees in Chemistry from Shandong University (Jinan, China), and Ph.D. degree in Electrical Engineering from Twente University (Enschede, the Netherlands) in 2009. After a postdoctoral research at MESA+ Institute of Nanotechnology in the Netherlands, she joined the faculty of South China Normal University in 2012. Her research interests lie in the fields of microfluidics and lab-on-a-chip. She has authored or co-authored more than 100 refereed journal papers with over 5000 citations, and has delivered over 50 invited talks/seminars in international/national conferences.

Abstract

Self-assembly has been recommended as a bridge tool bringing basic units to functional structures, and has attracted attentions from multidisciplinary fields. Droplet microfluidics offers a confined fluidic space with pL to nL volume, with controllable physical and chemical parameters for internal particle/molecule manipulation. In this presentation, I will present our recent findings of supraparticles constructed via microfluidic droplet confined particle assembly. The configurable structures of the supraparticles enable its applications in intelligent sensors for pH, ion, molecule and microorganism detection.

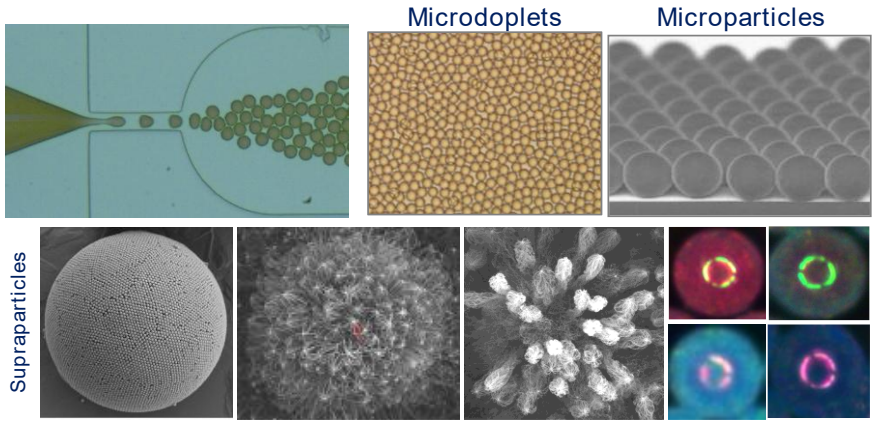

Figure 1. Droplet microfluidics for constructing supraparticles with hierarchical configurations. (a) Droplet generation at the flow focusing area in droplet microfluidic device. (b) Obtained droplets containing colloidal particles. (c) Obtained microparticles via solvent evaporation. (d) Obtained supraparticles with various hierarchical structures[1,2,3].

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2. J. Wang, L. Segerink, L. Shui,* and et al. " Mass Transport Determined Silica Nanowires Growth on Spherical Photonic Crystals with Nanostructure-Enabled Functionalities", *Small*, 16, 2001026 (2020).
3. X. Li, S. Huang, L. Shui*, and et al. "MoS_2 Loaded Cholesteric Liquid Crystal Microcapsules for NIR Responsive Thermochromism", Lab on a Chip, Accepted.

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Plenary Talk

Chairperson: Kiichi Sato

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[9budaVfT] **MOF Crystallography of Microgram-Scale Bioactive Molecules**

Masaki Kawano (Institute of Science Tokyo)

MOF Crystallography of Microgram-Scale Bioactive Molecules

Masaki KAWANO
Institute of Science Tokyo/TEKMOF Co., Ltd.

Biographical Sketch

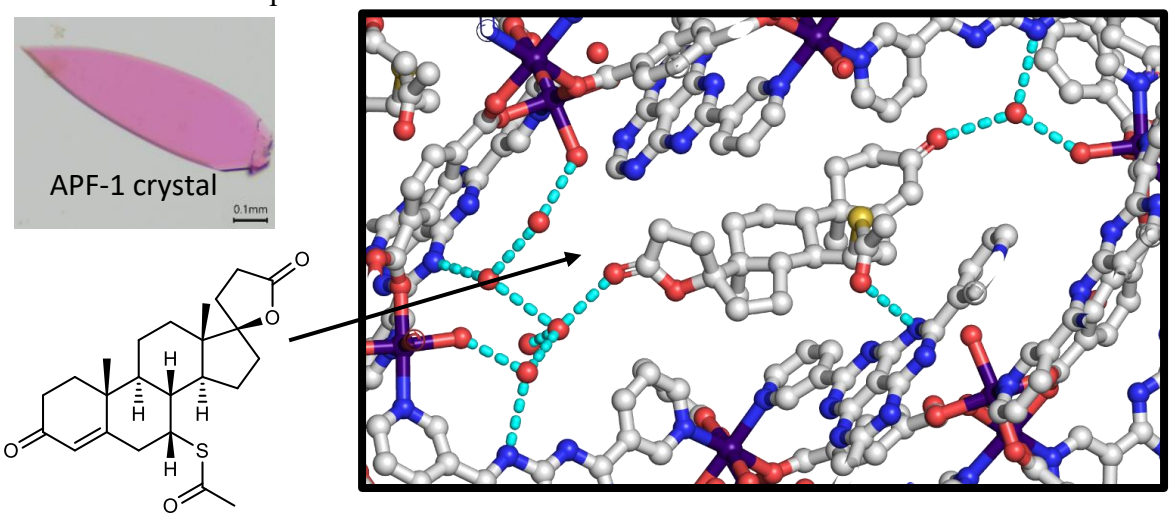
Waseda University, Department of Chemistry, Ph.D. (Science, 1993)
Associate Professor (2003-2009), Department of Applied Chemistry, The University of Tokyo. After serving as Professor, Department of Advanced Materials Science, POSTECH (2009-2015), in 2015, he was appointed professor at the Department of Chemistry, Tokyo Institute of Technology, where he currently holds the position.
Since 2024, he has been the founder and CSO of TEKMOF.
His research interests include Coordination chemistry, Supramolecular chemistry, MOF, In situ chemical crystallography, Crystalline-state photochemistry, ab initio powder X-ray crystallography.

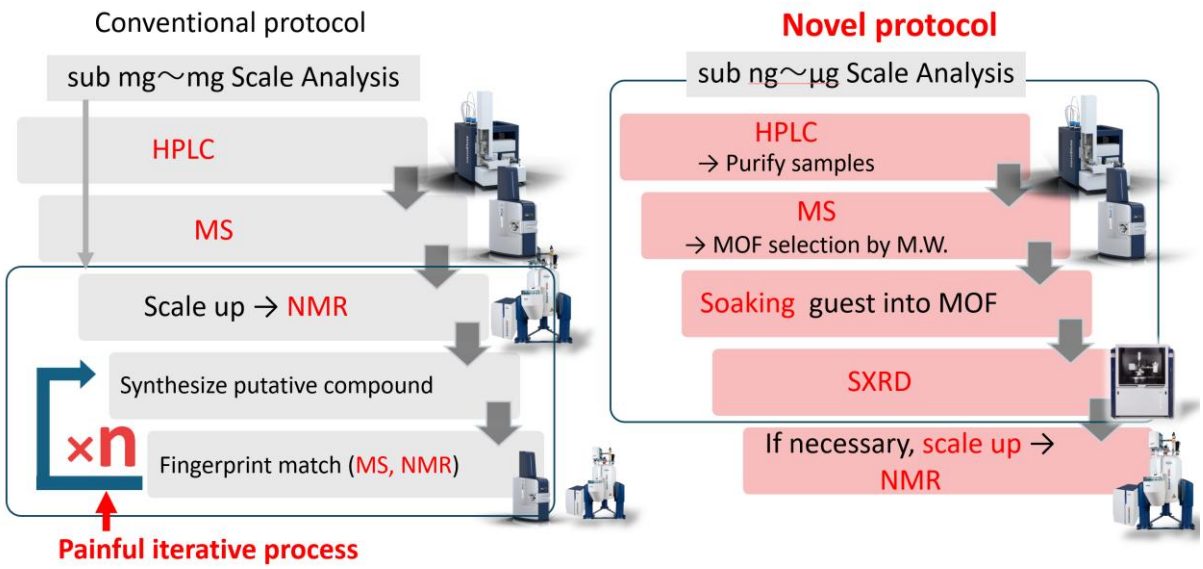
Abstract

We have developed metal–organic frameworks (MOFs) incorporating interactive ligands to trap metastable structures and construct responsive pore environments. An interactive ligand is defined as a bridging ligand bearing functional groups capable of engaging in supramolecular interactions. These ligands enable a range of fascinating functions, including kinetic trapping [1], selective guest recognition [2], ion conductivity [3], non-volatile memory storage [4], and more.

Notably, we have designed adaptable pores capable of visualizing natural products at atomic-level resolution as shown in Figure [5]. While the crystalline sponge method has proven effective for analyzing small molecules [6], it still faces several challenges, such as limitations in molecular size, chemical and physical stability, and issues arising from pseudo-symmetry.

To address these challenges, we are developing new MOF systems tailored for enhanced structural elucidation of natural products. In this presentation, we will share our recent progress, with a particular emphasis on the structural analysis of microgram-scale nucleophilic natural products and medium-sized molecules [7], and the use of a high-speed simulator called Matlantis for structural prediction.





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Plenary Talk

Chairperson: Deniel Citterio

[Plenary Talk] **From data accquisiton to knowledge generation: The trandformative role of artifical intelligence in analytical chemistry**

Pai-Shan Chen (National Taiwan University)

From data acquisition to knowledge generation: The transformative role of artificial intelligence in analytical chemistry

Pai-Shan CHEN
Graduate Institute of Toxicology, National Taiwan University College of Medicine, National Taiwan University, Taipei, Taiwan

Biographical Sketch

Professor Pai-Shan Chen is a Professor at National Taiwan University (NTU), Taiwan, and received her Ph.D. in Analytical, Environmental & Forensic Sciences from King's College London, UK. Her research focuses on mass spectrometry, analytical toxicology, artificial intelligence-assisted analytical chemistry, and the development of innovative LC–MS platforms for forensic, clinical, and environmental applications. Her research spans wastewater-based epidemiology, forensic toxicology, and clinical metabolomics, with recent efforts directed toward applying artificial intelligence to mass spectrometry data for rare disease diagnosis and biomarker discovery. She has been invited to present her work at major international conferences, including TIAFT, AOMSC, and CMSC Asia. Professor Chen served as the Taiwan Representative to the International Association of Forensic Toxicologists (TIAFT) and received the 2024 Young Scholar Award from the Taiwan Society for Mass Spectrometry (TSMS). Her current research explores how artificial intelligence can transform analytical chemistry from a data-generating discipline into a knowledge-generation science, with applications in metabolomics, biomarker discovery, clinical diagnostics, and autonomous analytical systems.

Abstract

Artificial intelligence (AI) is rapidly reshaping analytical chemistry by transforming how complex analytical data are translated into actionable knowledge. While advances in mass spectrometry, chromatography, and sensing technologies have greatly expanded analytical capabilities, the resulting data complexity has shifted the primary bottleneck from data acquisition to data interpretation. AI is driving a paradigm shift across mass spectrometry-based applications. In clinical metabolomics, machine learning models have enabled accurate diagnosis and classification of rare inherited metabolic disorders using urinary organic acid profiles, reducing reliance on expert interpretation. In untargeted metabolomics, AI-assisted platforms facilitate biomarker discovery, automate statistical analyses, improve feature prioritization, and accelerate knowledge extraction from large-scale datasets. Beyond data analysis, AI is increasingly contributing to analytical method development. Advances in generative AI and predictive modeling support data processing, visualization, and reporting, while also assisting in the prediction of feasible analytical strategies, optimization of experimental conditions, and acceleration of method development. By reducing technical barriers and minimizing trial-and-error experimentation, AI may enable analytical scientists to focus more directly on scientific questions and discovery. Recent advances in AI for Science suggest that artificial intelligence may increasingly participate in multiple stages of the scientific process, ranging from data interpretation and experimental design to knowledge discovery and decision support. More importantly, AI has the potential to redefine the role of analytical chemists. Historically, analytical laboratories have focused primarily on data generation, whereas transforming analytical data into scientific knowledge often required fragmented and labor-intensive workflows. AI-assisted systems may help integrate data acquisition, interpretation, and decision support within a more unified framework, potentially

accelerating discovery and improving analytical reproducibility. Looking ahead, the convergence of AI, advanced instrumentation, robotics, and intelligent sensing technologies may lead to autonomous analytical systems capable of supporting real-time decision-making and adaptive experimental design. Such developments could further shorten the path from data generation to scientific insight and expand the accessibility of advanced analytical technologies. The future analytical laboratory may evolve from a data-generating facility into an intelligent knowledge-generation system, where AI serves not merely as a computational tool but as a collaborative partner in scientific discovery.

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[Plenary Talk] **Computational and machine learning approaches for the identification of unknown chemicals by mass spectrometry**

Han Bin Ph (Sogang University)

Computational and machine learning approaches for the identification of unknown chemicals by mass spectrometry

Han Bin Oh
Department of Chemistry, Sogang University, Republic of Korea

Biographical Sketch

Professor Han Bin Oh received his B.S. degree from Seoul National University in 1993 and his Ph.D. from the University of Toronto in 2001. He conducted postdoctoral research at Cornell University fro 2001 to 2003 and has been a faculty member at Sogang University since 2003. His reseach forcuses on mass spectrometry, machine learning, and toxicology. He served as Editor-in-Chief of Mass Spectrometry Letters (2018-2019) and the Journal of the Korean Chemical Society(2023-2024). He also served as Executive Vice President for General Affairs of the Korean Chemical Society (2024-2025). His work integrates adevance analytical Sciences with data-driven approaches to address challenges in chemistry and life sciences.

Abstract

The chemical space of potential organic compounds is extraordinarily vast, encompassing far more molecules than can be experimentally characterized. In contrast, tandem mass spectrometry (MS/MS) data are available for only a small fraction of known chemicals, creating a significant bottleneck in the identification of unknown compounds encountered in chemical, pharmaceutical, forensic, and toxicological analyses. Although substantial efforts have been devoted to addressing this challenge, the reliable identification of unknown chemicals remains one of the most important unsolved problems in mass spectrometry.

Our research focuses on narrowing the relevant chemical space and leveraging computational and machine learning approaches to facilitate the identification of unknown chemicals. In particular, we develop strategies for generating virtual chemical libraries, predicting tandem mass spectra using machine learning models, and constructing virtual MS/MS databases that can be used for the annotation and identification of previously uncharacterized compounds.

A major application area of this work has been the identification of emerging illicit substances, including novel phosphodiesterase type 5 (PDE5) inhibitor analogs and new psychoactive substances (NPS), in collaboration with the Korean Ministry of Food and Drug Safety (MFDS). By exploiting the relatively constrained chemical spaces associated with these compound classes, we generate virtual candidate structures, develop machine learning-based MS/MS prediction models, and construct virtual spectral databases to support the detection and identification of compounds for which experimental reference spectra are unavailable.

Recent advances in generative modeling have opened new opportunities for exploring previously uncharted regions of chemical space. We are actively investigating how these emerging technologies can be integrated with mass spectrometry workflows to further improve the identification of unknown chemicals. In this symposium, we will share our recent developments, methodologies, and applications, highlighting the potential of computational

and machine learning approaches to advance unknown chemical identification by mass spectrometry.

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