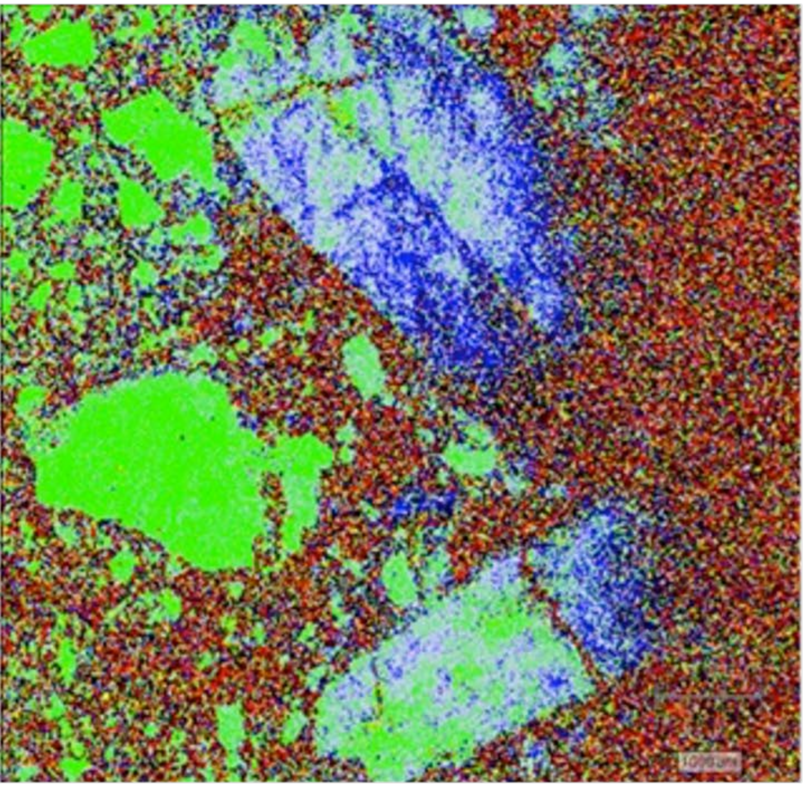
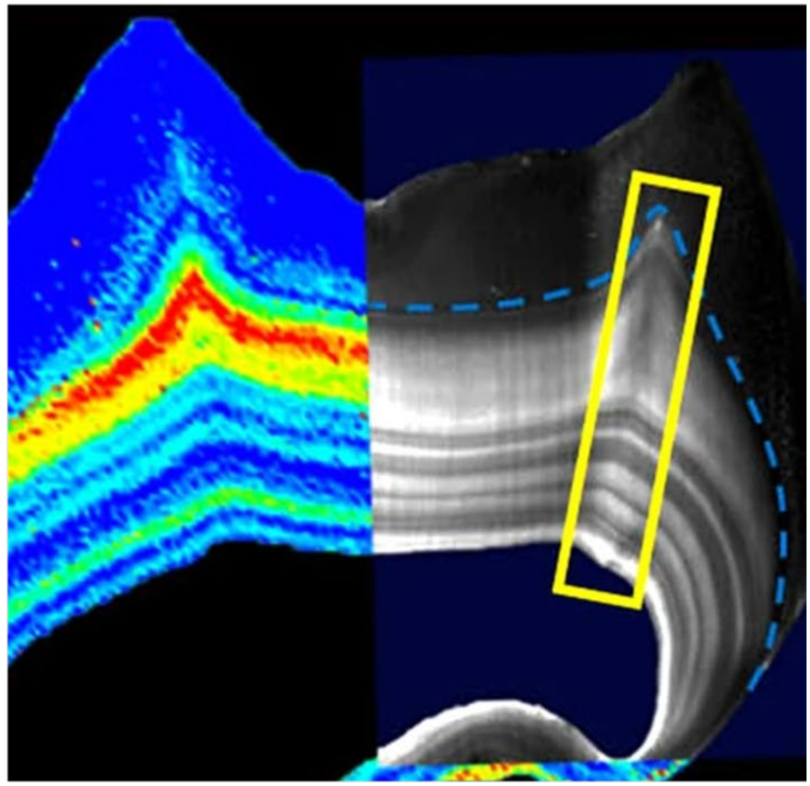
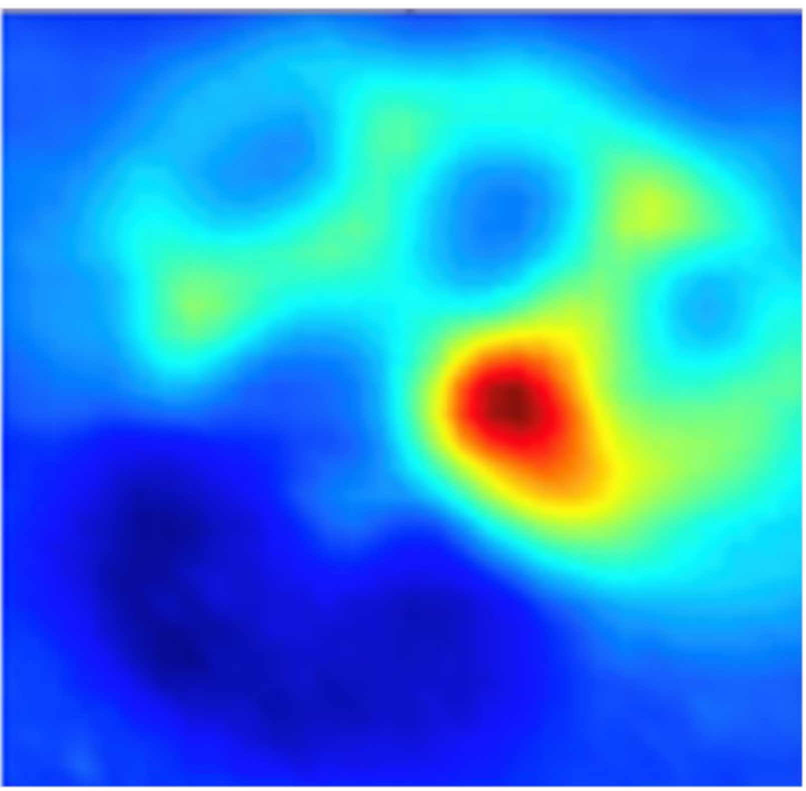
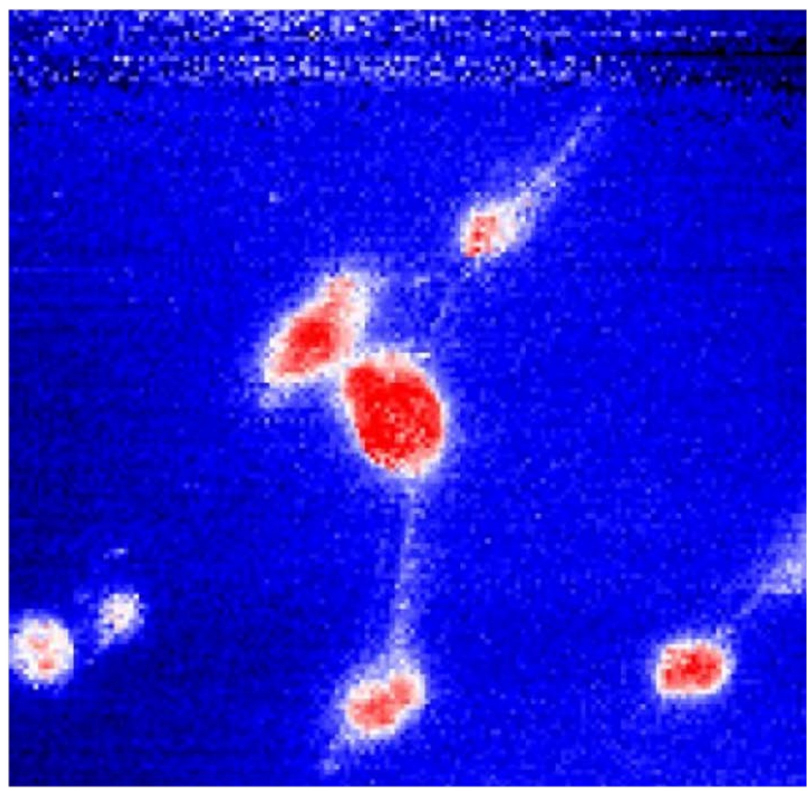

2026 Symposium

Hosted by Sydney Analytical
8–10 July, 2026

Preface

The Sydney Analytical Vibrational Spectroscopy Facility team welcome you to the University of Sydney.

We extend a warm welcome to all delegates joining us from across Australia and internationally, both in person and remotely. Your participation reflects the strength and diversity of the vibrational spectroscopy community, and we are delighted to host you for three days of scientific exchange, collaboration, and inspiration.

This year's symposium, held from 8–10 July 2026, brings together innovation across materials, life sciences, and environmental research enabled by advanced vibrational spectroscopy. The program highlights emerging approaches, new analytical capabilities, and real-world applications, with a strong focus on how these techniques are being translated into impactful research outcomes.

Program highlights include:

- A Keynote Lecture by Prof. Natalie Sims (*St. Vincent's Institute of Medical Research and the University of Melbourne*), whose work uses advanced vibrational spectroscopy to investigate bone matrix composition, mineralisation, and skeletal health across the lifespan.
- Invited presentations from distinguished speakers including Dr Ross Graham (*Curtin University*), A/Prof. Thomas Rodemann (*University of Tasmania*), Dr Hayley Green (*Western Sydney University*), and Dr Richard Wuhrer (*Western Sydney University*), reflecting the breadth of vibrational spectroscopy across biological, environmental, and materials science applications.
- A diverse program of oral presentations and lightning talks, showcasing innovative research and practical insights across materials, life sciences, environmental monitoring, and cultural heritage applications.
- A dedicated MicroparticlesAI workshop, led by Dr Benedikt Hufnagl, exploring chemometric and machine learning approaches for advancing microplastics analysis and data reliability.

We are especially proud to support emerging researchers. Many presentations throughout the program are delivered by postgraduate students 🧑‍🎓, highlighting the next generation of scientists contributing to advances in vibrational spectroscopy.

We gratefully acknowledge the support of our sponsors and exhibitors, whose contributions make this symposium possible and help foster the innovation, collaboration, and exchange that underpin our community.

Finally, thank you for being part of the 2026 Sydney Analytical Vibrational Spectroscopy Symposium. We hope the program provides you with new ideas, practical tools, and meaningful connections that will enrich your research and professional journey

Sydney Analytical

Sydney Analytical is the University of Sydney's core research facility for chemical and materials analysis, offering world-class expertise and instrumentation across vibrational spectroscopy, X-ray techniques, and surface analysis. The facility supports researchers from academia, industry, and government, enabling cutting-edge investigations in fields ranging from biomedical science and environmental chemistry to cultural heritage and advanced materials.

The Vibrational Spectroscopy Facility, which is hosting the Symposium, provides access to state-of-the-art FTIR, Raman, and NIR spectroscopy, including imaging and mapping capabilities. Staffed by experienced scientists, the facility offers tailored support for experimental design, data interpretation, and method development.
Sydney Analytical is committed to fostering collaboration, innovation, and education through workshops, training programs, and symposia like this one. Whether you're solving complex analytical problems or exploring new frontiers in spectroscopy, Sydney Analytical is your partner in discovery.

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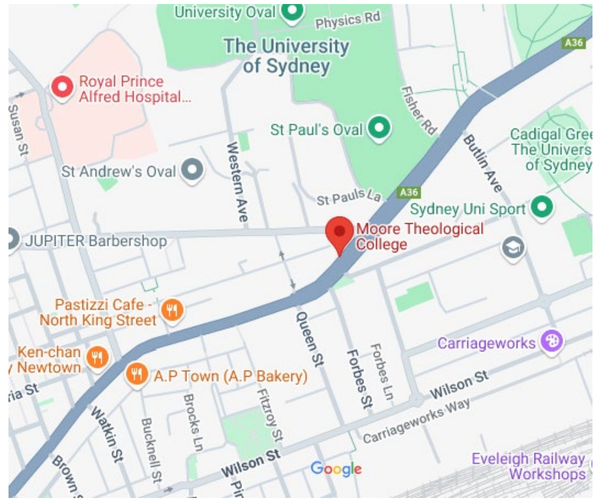
General Information

Venue Location



The venue for the 2026 Sydney Analytical Vibrational Spectroscopy Symposium is Moore College, located at Level 5, Room 503 (Auditorium), 1 King Street, Newtown, NSW 2042, Australia

Registration

Registration and arrival will begin at **9:00 am on Wednesday 8th July 2026**.

Meals

Catering, including tea and coffee, will be provided on-site each day.

Directions

Sydney Trains

- Use an Opal card for all Sydney Trains or tap on/off with your credit card.
- Closest stations: Redfern, Newtown, or Central (via bus).
- Walking directions from Newtown: 15 minutes, right from exit, up King Street.
- Walking directions from Redfern: 15 minutes, left from exit, down Lawson Street, left on Abercrombie Street, right on Codrington Street, past Sydney Uni sports complex, left on Darlington Street, cross King Street, towards Newtown/Enmore.
- Plan trips with www.transportnsw.info for additional bus options.

Sydney Buses

- Opal card required for Sydney Buses or tap on/off with credit card.
- Key buses: 423, 426, 428, and Metrobus 430 from various city locations.
- Alight at King Street near Carillon Avenue, walk past the bus stop to 1 King Street.

Driving

- No off-street visitor parking is available at Moore College.
- Limited metered street parking is available.
- Public transport is recommended the closest bus stop is opposite to 1 King Street.

Acknowledgement of Sponsors

We're incredibly thankful to our sponsors whose generous support has made the 2026 Sydney Analytical Vibrational Spectroscopy Symposium a reality. Events like this thrive on collaboration, and we couldn't bring together such a vibrant community of researchers, speakers, and innovators without you.

A heartfelt thank you to:

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Warsash Scientific

Thank you for your continued support of vibrational spectroscopy and scientific exchange. By presenting your work and connecting with emerging and established researchers, you contribute to the innovation and collaboration that underpin our field.

We look forward to a rewarding week of science, learning, and collaboration.

TIMETABLE

Day 1 – Wednesday July 8

Time	
9:00 – 9:15	Registration & Arrival
9:15 – 9:30	Opening Address & Welcome
9:30 – 10:30	*Keynote Speaker:* Natalie Sims, *St. Vincent's Institute of Medical Research and the University of Melbourne*, – Using vibrational spectroscopy to study bone matrix composition and mineralisation.
10:30 – 11:00	*Morning Tea*
Session 1	**Materials**
11:00 - 11:20	🧑‍🎓 Peter Leung, *School of Physics, The University of Sydney* - Ammonium-Free-Layered-Perovskites with Alternating Cations in the Interlayer for Wide-Bandgap Solar Cells.
11:20 - 11:40	Anastasiia Tukova, *School of Natural Sciences, Macquarie University*: Label-free SERS detection of biological analytes.
11:40 - 12:00	Neeha Velagapudi and Karen Wilcox, *Australian National Maritim Museum*: NIR Spectroscopy for rapid, non-invasive analysis of cellulose nitrate and cellulose acetate negatives.
12:00 - 12:20	☀️ Stephanie Le Strange, *Metrohm Australia*: Spectroscopy Technologies and Applications
	Official Welcome
12:20 – 12:30	Pro-Vice Chancellor of Research Infrastructure (PVCRI) Prof. Simon Ringer
12:30 – 1:30	*Lunch*
Session 2	**Materials**
1:30 – 1:50	🧑‍🎓 Simran Sethi, *School of Chemical and Biomolecular Engineering, The University of Sydney*: Quantifying Carbonate and Hydroxide Phases in Carbon Mineralisation Products using TGA-FTIR. (presented by Majharul Haque Khan)
1:50 - 2:10	Shamim Sharhrokhi, *Anton Paar Australia & New Zealand Pty. Ltd.*: Raman on the Line: Real-Time Crystallinity Monitoring in PEEK Film Extrusion.
2:10 - 2:30	Yan Lu, *Biomedical Engineering, University of Sydney*: Plasmonic Skin as a Wearable SERS Substrate for Direct Chemical Identification.
2:30 - 2:35	🧑‍🎓 ⚡ Sophie Cottam, School of Biomedical Engineering, University of Sydney: Lasers for Lasers: Raman Spectroscopy of Laser-Induced Graphene Fabrication.
2:35 - 2:40	⚡ Ali Ibrahim, *Chau Chak Wing Museum, University of Sydney*: An in-depth analysis of ancient Egyptian cartonnage using Optical Photothermal IR (O-PTIR) Spectroscopy.
2:40 - 3:10	*Afternoon Tea*
Session 3	**Tour**
3:10 - 4:30	Facility Tour

⚡ - Lightning Presentation (5 Mins); 🧑‍🎓 - Student Presentation; ☀️ - Sponsor Presentation

Day 2 – Thursday July 9

Time	
9:00 – 9:20	Registration & Arrival
Session 4	**Life Sciences**
9:20 – 9:50	*Invited Speaker*: Ross Graham, *Curtin Medical Research Institute, Curtin University*: Live cell imaging using time-lapse FTIR spectroscopy.
9:50 – 10:10	Graeme Batten, *School of Life and Environmental Sciences, University of Sydney*: Near infrared spectroscopy of two highly correlated constituents in wheat grains.
10:10 – 10:30	🧑‍🎓 Luke Pevey, *Sydney Pharmacy School, The University of Sydney*: Rapid Biochemical Profiling of Probiotic EVs Using High-Throughput FTIR Spectroscopy.
10:30 – 11:00	*Morning Tea*
Session 5	**Life Sciences**
11:00 - 11:30	*Invited Speaker*: Hayley Green, *School of Science, Western Sydney University* – Assessment of Late Postmortem interval of Skeletal Remains using Raman and FTIR Spectroscopy.
11:30 - 11:50	🧑‍🎓 Xiaorui Cao, *School of Biomedical Engineering, University of Sydney*: SERS-based plasmonic biosensor for 3D cardiac model metabolites monitoring.
11:50 - 12:10	🧑‍🎓 Cameron Issacs, *College of Science and Engineering, Flinders University*: Low-Wavenumber Characterisation of Multi-Substituted Apatites.
12:10 – 1:00	*Lunch*
Session 6	**Environment**
1:00 – 1:30	*Invited Speaker*: Thomas Rodemann, *Central Science Laboratory, University of Tasmania*– From TerraSpec to Predictive Mineral Intelligence: Quantifying Infrared Spectroscopy for Mining.
1:30 - 1:50	Rachel Yamamoto, *School of Life and Environmental Sciences, University of Sydney*: Spatial Differences in Aggregate Stabilised Mineral Associated Organic Matter Under Three Agricultural Soils.
1:50 - 2:10	🧑‍🎓 Christine Fink, *School of Civil Engineering, University of Sydney*: Assessing Focus Accuracy and Substrate Effects in FPA-Based Microplastic Analysis Comparing LUMOS II and SPERO Systems.
2:10 -2:30	🌞 Koman Tam, *Bruker Pty Ltd*: Environmental particles Detection by QCL IR imaging and NEMS-FTIR Spectroscopy.
2:30 - 2:35	⚡ Kim Tran, *Sydney Institute of Agriculture and the School of Life and Environmental Sciences, University of Sydney*: From One Soil Spectrum to Multiple Environmental Information: Mid-Infrared Spectroscopy for Soil Biology, Carbon, and Microplastics.

2:35-2:55	Benedikt Hugnafl, *Hufnagl Chemometrics GmbH*: Toward Reliable Microplastics Data: Challenges in Spectroscopic Analysis and Machine Learning.
2:55 – 3:15	*Tea + Coffee Break*
Session 7	
3:15 – 3:45	<u>*Invited Speaker*</u>: Richard Wuhrer, *Advanced Materials Characterisation Facility, Western Sydney University* – Next Generation of Instruments Required - Combined and Correlative SEM, EDS, XRM, CL, Raman and Optical System (Colour-CL-GSR System) for Gunshot Residue and Mineralogical Analysis
3:45 – 4:05	🌟 Mustafa Kansiz, *Photothermal Spectroscopy Corp.*: Multimodal high-speed laser-scanning submicron Infrared (O-PTIR) and Stimulated Raman (PT-SRS) Platform for Real-time Label-free Chemical Imaging
4:05 – 4:25	🌟 Derek Huxley, *Warsash Scientific*: Advanced Instruments for Research, Safety and Security.
4:30 - 6:00	*Rooftop canapes*

⚡ - Lightning Presentation (5 Mins); 🧑‍🎓 - Student Presentation; 🌟 - Sponsor Presentation

Day 3 – Friday July 10

Time	
9:00 – 11:00	Benedikt Hugnafl, *Hufnagl Chemometrics GmbH*
	MicroparticlesAI Workshop – Session 1:
	Covers key concepts in chemometrics, including the differences between spectral library search and machine learning models, strategies for building representative training datasets, and the role of iterative improvement and domain shift.
11:00 – 11:30	*Morning Tea*
11:30 – 1:30	**MicroparticlesAI Workshop – Session 2:**
	Presents microparticlesAI and its application in real-world analysis.
1:30 – 2:15	Symposium Closing and Lunch

KEYNOTE SPEAKER

USING VIBRATIONAL SPECTROSCOPY TO STUDY BONE MATRIX COMPOSITION AND MINERALISATION

Natalie A. Sims

St. Vincent's Institute of Medical Research, 9 Princes St, Fitzroy, Australia; Department of Medicine at St. Vincent's Hospital, The University of Melbourne, Australia; Faculty of Health Sciences, Australian Catholic University, Melbourne, Australia

Bone formation is a continuous process occurring across the lifespan: from embryogenesis and skeletal growth through to the lifelong cycle of renewal known as remodelling. The bone matrix itself is a composite material comprising type I collagen fibres reinforced by bioapatite crystals, and the relative quantities, organisation, and maturation of these components are determinants of bone mechanical strength. Understanding how this composition is regulated, and how it changes with age or disease, is therefore central to understanding skeletal fragility.

Our laboratory has employed a suite of vibrational spectroscopic techniques to interrogate bone matrix composition at the tissue level. Using synchrotron-based Fourier-transform infrared microspectroscopy (sFTIRM) and polarised FTIRM (2-angle), we demonstrated in genetically modified mouse models that the signalling protein EphrinB2 governs three distinct aspects of bone mineralisation: the rate of mineral accrual, the degree of carbonate substitution within the bioapatite lattice, and the compaction of collagen fibres within the bone matrix. These findings established a molecular link between cell signalling and the physicochemical properties of bone material.

Since murine bone lacks the osteonal structures that comprise the bulk of adult human cortical bone, we have more recently studied bone composition in cadaveric human specimens from the Melbourne Femur Research Collection, representing healthy bone from a modern urban population. We developed a framework, using sFTIRM and back-scatter electron imaging to identify specific stages of bone maturity. This is revealing differences in how bone matrix is produced and mineralised between young (19–35 years) and older (71–95 years) women, measured by sFTIRM, 4-angle polarised FTIRM, and Raman spectroscopy. These complementary methods provide a multidimensional picture of how ageing influences the bone formation process. The combined data will be presented, with a focus on how spectroscopic approaches are informing our understanding of the processes that control bone material composition and strength.

Biography

Professor Sims directs the Bone Cell Biology and Disease Unit at St. Vincent's Institute of Medical Research and is a Professorial Fellow at The University of Melbourne and Australian Catholic University. She leads a team studying the cellular interactions responsible for development, maintenance, and strength of the skeleton, using genetically altered mouse models, in vitro systems, and human specimens and methods that assess bone mass, organisation and composition, including spectroscopy. Her work has been recognised by the International Bone and Mineral Society Herbert A Fleisch Award (2013), the American Society of Bone and Mineral Research Fuller Albright (2010) and Paula Stern (2020) Awards, and the Australia and New Zealand Bone and Mineral Society (ANZBMS) Career Achievement Award (2023). She has served as President of the ANZBMS and is a Deputy Editor of the Journal of Bone and Mineral Research and serves on the Editorial Board of the Journal of Biological Chemistry.

SESSION 1 - MATERIALS

AMMONIUM-FREE-LAYERED-PEROVSKITES WITH ALTERNATING CATIONS IN THE INTERLAYER FOR WIDE-BANDGAP SOLAR CELLS

Tik Lun Leung, Anita Ho-Baillie

School of Physics, The University of Sydney, Sydney, NSW, Australia
Sydney Nano, The University of Sydney, Sydney, NSW, Australia

The desire to mitigate climate change by decarbonizing the electricity sector has led to an unprecedented demand for renewable energy. While silicon solar cells currently dominate the market, they are rapidly approaching their theoretical power conversion efficiency limits, necessitating the development of multijunction (tandem) solar cells that have efficiency limits at 45% for double junctions and 51% for triple junctions. Multijunction solar cells stack wide band gap solar cells on top of narrow bandgap ones such that they work in tandem. The wide bandgap cell is responsible for efficiently harnessing the “bluer” portion of the solar spectrum for electrical energy generation, while the and the narrow bandgap cell is responsible for the “redder” portion of the spectrum.

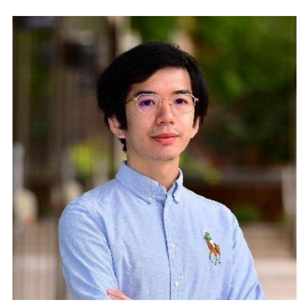
Metal halide perovskite solar cells are promising for multijunction solar cells due to their rapid improvements in demonstrated power conversion efficiencies and their bandgap tunability. However, many of the state-of-the-art wide bandgap perovskite cells consist of multiple halide components, which are susceptible to segregation under illumination, compromising long-term operational stability. Layered metal halide perovskites can achieve wide bandgap without halide mixing through dielectric and quantum confinement effects while simultaneously enhancing stability.

Among layered metal halide perovskites, the alternating cation interlayer (ACI) family typically exhibit small interlayer spacing, which lowers exciton binding energy and promotes free carrier generation, favorable for photovoltaic devices. However, most reported ACI phase perovskites incorporate volatile methylammonium (MA) cations, susceptible to instability. Here, we report an ammonium-free-ACI $(GA)(Cs_xFA_{1-x})_2Pb_2I_7$ perovskite that produces a wide-bandgap of 2.1 eV without halide mixing. The mechanism of n=2 and higher n phases is found to be dependent on the molar ratio of cesium (Cs) and formamidinium (FA) in the A-site, elucidated via the use of scanning near-field optical microscopy (SNOM) and X-ray diffraction supported by Sydney Analytical.

The corresponding wide bandgap device produces notable power conversion efficiency (PCE), which is to date the highest for n = 2 layered perovskite solar cells. The stability of encapsulated cell also outperforms reported perovskite solar cells of the same bandgap, highlighting the value of developing ammonium-free iodide 2D ACI perovskites.

Biography

Dr. Tik Lun (Peter) Leung is a postdoctoral researcher in the School of Physics at the University of Sydney, where he also earned his PhD in 2026. His doctoral thesis is on low dimensional metal halide perovskites for optoelectronics. Currently, his research focuses on halide perovskite field-effect transistors (FETs) for neuromorphic applications.



LABEL-FREE SERS DETECTION OF BIOLOGICAL ANALYTES

Anastasiia Tukova

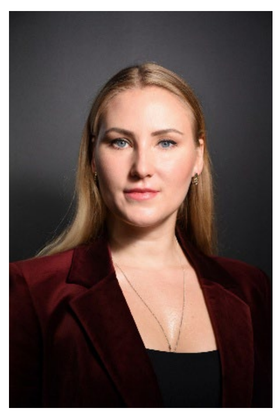
School of Natural Sciences, Faculty of Science and Engineering, Macquarie University, Sydney, NSW 2109, Australia

Surface-enhanced Raman scattering (SERS) is a powerful vibrational spectroscopic technique that enables highly sensitive, label-free molecular detection by amplifying Raman signals at plasmonic nanostructures. As a biospectroscopic approach, SERS can probe native biochemical signatures from complex biological systems, including proteins, nucleic acids, extracellular vesicles, and cells, without external labels. However, reliable and reproducible label-free SERS remains challenging because signal generation depends on nanostructure geometry, surface chemistry, analyte–surface interactions, and measurement conditions. These factors strongly affect sensitivity, spectral quality, molecular selectivity, and preservation of native biomolecular information.

This work investigates the fundamental interactions between plasmonic nanostructures and biologically relevant targets, including proteins, nucleic acids, extracellular vesicles, and cells, to establish standardized methodologies for label-free SERS-based biospectroscopy. Particular attention is given to how nanoparticle design, substrate characteristics, and experimental parameters influence analyte adsorption, plasmonic enhancement, and spectral reproducibility. By systematically examining these relationships, the study identifies conditions that maximize sensitivity while preserving molecular specificity and minimizing artefacts, variability, and substrate-induced bias.

The findings provide a biospectroscopic framework for the rational design of SERS platforms tailored to biological systems, where maintaining native biomolecular signatures is essential for accurate structural, functional, and diagnostic interpretation. This study defines key design and measurement principles required for robust, reproducible, and analytically meaningful label-free SERS biospectroscopy. By advancing standardization in substrate design, sample preparation, and spectral acquisition, this work supports the development of SERS as a reliable platform for probing biomolecular structure, function, and dynamic interactions, with implications for biosensing, diagnostics, liquid biopsy analysis, and studies of complex biological systems.

Biography



Dr Anastasiia Tukova is a Macquarie University Lighthouse Fellow working at the interface of plasmonic nanotechnology, optical spectroscopy and translational biosensing. Her research focuses on designing and functionalising gold nanostructures for sensitive detection of disease-associated biomarkers in liquid biopsy samples. She specialises in Surface-Enhanced Raman Spectroscopy (SERS) and Raman and, biointerface chemistry, protein corona analysis and chemometric data interpretation.

Dr Tukova completed her PhD in Chemistry and Biomolecular Sciences at Macquarie University in 2025 and has developed an interdisciplinary profile spanning nanomaterials, analytical chemistry, spectroscopy and point-of-care diagnostics. Her work has resulted in peer-reviewed publications, a book chapter, grants, awards and intellectual property related to plasmonic nanosensor platforms. She also contributes to teaching, mentoring and spectroscopy training, and is co-founder of iNanoDx, a start-up translating nanosensor technologies into accessible cancer diagnostic solutions for future clinical implementation and equitable healthcare worldwide.

NIR SPECTROSCOPY FOR RAPID, NON-INVASIVE ANALYSIS OF CELLULOSE NITRATE AND CELLULOSE ACETATE NEGATIVES

Neeha Velagapudi and Karen Wilcox

Australian National Maritime Museum, Sydney, NSW, Australia.

Staff working with historic collections need techniques to rapidly differentiate objects made with cellulose nitrate or cellulose acetate to apply appropriate preservation strategies. Nitrate and acetate negatives are inherently malignant compared to later polyester films, and they emit corrosive gases as they degrade. Nitrate films also have additional hazards, classed as a flammable solid.

Using visual, historical, or contextual cues for film identification is time consuming and relies on staff expertise. Spectroscopic analysis in the Mid Infrared (MIR) range is a common technique. However, mounting samples on the instrument for a clear measurement can be difficult, and interpretation can be complicated by the layered composite structure of negatives. Novel methods are being developed to improve analysis towards this goal of rapid, non-destructive identification by collection staff with limited experience in spectroscopic analysis.

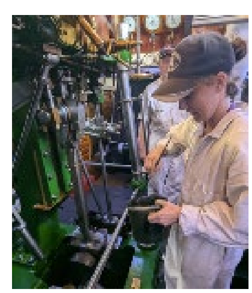
Conservators at the Australian National Maritime Museum (ANMM) recently trialed the use of a FT-NIR spectrometer (MPA III, Bruker Optiks GmbH) for film analysis, based on an observation by Carter (2019) that there were distinct spectral features in the range 6,500-4,000cm^{-1} for the different film types when comparing instruments across the MIR and Near Infrared (NIR) wavelengths.

This presentation will share the results of our trial and discuss the benefits of using NIR analysis with respect to object safety, the speed of analysis, and the distinct features allowing for confident visual interpretation of the three types of film base. We will also examine ways to further refine this method, consider its application to identifying other types of objects likely made of these materials, and question how to increase the accessibility of this technique, such as through handheld NIR devices.

Biography

Neeha Velagapudi is an Objects Conservator at the Australian National Maritime Museum, with a focus on preparing malignant plastic collection items for long term cold storage. Prior to her role at ANMM, her work was based in Aotearoa New Zealand, both in a private practice and at Canterbury Museum. While there she worked on significant projects such as the conservation of whare whakairo, leading an outreach project to support smaller museums in the Canterbury region, and research into the use of Lascaux 303HV to secure displayed collection items in earthquake prone areas.

Karen Wilcox is an Objects Conservator at the Australian National Maritime Museum. She was introduced to FT-IR spectroscopy whilst researching painted aircraft markings during a Graduate Fellowship at the Smithsonian National Air and Space Museum, and she has also previously worked at the Australian War Memorial, the State Library of New South Wales, and private practices in Australia and New Zealand. Her interests include the conservation of large technology, the maintenance of functional objects, and complex modern materials.



SPECTROSCOPY TECHNOLOGIES AND APPLICATIONS

Stephanie Le Strange

Metrohm Australia

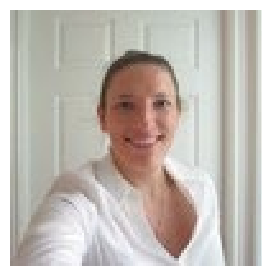
Metrohm Australia offer a comprehensive portfolio of analytical equipment from titration to electrochemistry, ion chromatography and spectroscopy. Metrohm Spectro develops and manufactures high-performance stabilized lasers, modular spectrometers, and handheld and benchtop Raman analyzers. These Raman solutions support a wide range of industries, including research, pharmaceuticals, food and beverage, defence and security, and advanced materials.
This presentation will showcase Metrohm Spectro's extensive Raman instrumentation portfolio, from robust handheld systems designed for field and industrial applications to advanced benchtop laboratory instruments. We will also explore the flexibility of Metrohm's modular 'DIY' Raman platforms, which provide tailored solutions for research groups and custom analytical applications.

High quality and innovation are key drivers of the development and production process at Metrohm Spectro. These innovations translate into enhanced sensitivity, selectivity and overall analytical performance for your Raman measurements.

We will then explore how our instrumentation has been used in some key applications, demonstrating the versatility of Raman spectroscopy across research and industry. Topics will include how Raman is used in the characterization of carbon-based materials and the integration of electrochemical analysis with Raman spectroscopy for spectroelectrochemistry experiments.

Biography

Stephanie LeStrange is the Territory Manager for NSW (South) at Metrohm bringing together extensive laboratory experience and a passion for helping customers solve analytical challenges. With 14 years of hands-on commercial laboratory experience in both the environmental and pharmaceutical industries, she understands the realities of laboratory operations. This translates to a practical understanding of analytical workflows, quality assurance and the challenges faced by scientists and laboratory professionals.



At Metrohm, Stephanie partners with laboratories across a diverse range of industries, helping customers unlock greater accuracy, productivity, and confidence in their analytical results through innovative instrumentation.

SESSION 2 - MATERIALS

QUANTIFYING CARBONATE AND HYDROXIDE PHASES IN CARBON MINERALISATION PRODUCTS USING TGA-FTIR

Simran Sethi[1], Majharul Haque Khan[2], Marjorie Valix[1], David K. Wang[1]

[1]*School of Chemical and Biomolecular Engineering, University of Sydney, Sydney, Australia*

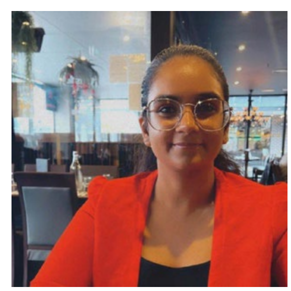
[2]*Sydney Analytical, The University of Sydney, Sydney, NSW, Australia.*

Carbon mineralisation offers a pathway for permanent CO_2 storage by converting reactive alkaline materials, such as Mg-rich mine tailings, into stable solid carbonate products. However, characterising these products is challenging because precipitation often produces complex mixtures of crystalline, poorly crystalline, hydrated, hydroxide, and carbonate-bearing phases. Conventional techniques such as XRD, ATR-FTIR, and SEM-EDS provide valuable structural and morphological information, but quantitative interpretation is limited when phases overlap, are amorphous, or occur in low abundance.

This presentation describes the use of thermogravimetric analysis coupled with Fourier-transform infrared spectroscopy (TGA-FTIR) as a quantitative tool for determining solid product composition in carbon mineralisation experiments. The method combines thermal mass-loss profiles with evolved-gas FTIR signals, particularly H_2O and CO_2 bands, to distinguish hydroxide and carbonate decomposition events. Calibration and integration of these regions enabled estimation of carbonate and hydroxide contributions across catalyst-assisted carbonation experiments, specifically in Mg, Fe(II), Fe(III), Al, Ca and mixed metal environments.

The results show that TGA-FTIR can reveal shifts between hydroxide-dominated and carbonate-bearing products, support mass-balance calculations, and validate trends that are difficult to resolve by other solid characterisation techniques. Overall, this work demonstrates TGA-FTIR as a practical, information-rich approach for quantifying complex mineral carbonation products and linking solid composition to process performance.

Biography



Simran Sethi is a PhD candidate in Chemical Engineering, with research focused on carbon mineralisation using magnesium-rich mine tailings. Her work investigates how alkaline industrial residues can be converted into stable carbonate products for permanent CO_2 storage, with a particular focus on linking process conditions to solid product formation and composition.

Simran's research combines leaching, carbonation, and precipitation experiments with a range of characterisation techniques, including XRD, SEM-EDS, ATR-FTIR, and TGA-FTIR. A key part of her thesis has involved developing quantitative approaches to interpret complex mineral systems for predictive modelling. Through this work, Simran aims to improve the reliability of characterisation methods used to assess carbon mineralisation performance and long-term CO_2 storage potential.

RAMAN ON THE LINE: REAL-TIME CRYSTALLINITY MONITORING IN PEEK FILM EXTRUSION

Shamim Shahrokhi

Anton Paar Australia & New Zealand Pty. Ltd., North Ryde NSW 2113

Real-time control of crystallinity is critical for high-performance polymer films, particularly Polyether ether ketone (PEEK), where molecular ordering determines thermal, mechanical, chemical, and dimensional performance. This presentation explores how Raman spectroscopy can be integrated directly into a film extrusion line to quantify crystallinity as the process runs. A Raman spectrometer with a fiber probe mounted on a film haul-off unit records non-contact spectra of extruded PEEK after the cooling drums. Complementary Differential Scanning Calorimetry (DSC) measurements provide reference crystallinity values, enabling calibration of a Raman model based on crystallinity-sensitive PEEK bands. Once calibrated, the model tracks crystallinity continuously and reveals how draw-off speed changes drive structural evolution: crystallinity increases strongly above about 1.5 m/min, plateaus at higher draw-off speeds, and shows unstable behavior at lower speeds. This highlights how in-line vibrational spectroscopy can identify critical processing windows, support faster method development, reduce waste, and provide a practical foundation for closed-loop quality control in extrusion.

Biography

Dr. Shamim Shahrokhi is a Technical Sales Specialist in Characterisation at Anton Paar Australia and New Zealand. Her Characterisation portfolio includes Mechanical Surface Testing, Raman Spectroscopy, FTIR, SAXS and XRD. She has been responsible for technical support, application testing, and sales for different product lines since 2022. She holds a PhD in Materials Science and Engineering from the University of New South Wales (UNSW) and has experience in temperature-dependent XRD analysis, electrochemistry, and hardness testing of materials.

PLASMONIC SKIN AS A WEARABLE SERS SUBSTRATE FOR DIRECT CHEMICAL IDENTIFICATION

Yan Lu

Biomedical Engineering, The University of Sydney, Sydney, NSW, Australia.

Surface-enhanced Raman spectroscopy (SERS) offers molecular fingerprint information for trace chemical identification, but translating SERS from laboratory substrates to real-world surfaces remains challenging. Many practical analytes, such as pesticide residues, are distributed on rough, curved, porous, or topologically complex interfaces, where conventional rigid and flat SERS substrates cannot form intimate contact for efficient sampling. Here, we present a wearable plasmonic skin (P-skin) realize direct chemical collection and on-site SERS detection via a simple touch.

The P-skin is constructed from a Janus gold nanocube–nanostar plasmonic array embedded in an elastic PDMS matrix. This asymmetric architecture combines mechanical flexibility, fingertip wearability, and strong plasmonic enhancement: the PDMS support enables conformal contact with irregular surfaces, while the Janus Au nanostructure provides dense electromagnetic hot spots for Raman signal amplification. Coupled with a portable hand-held Raman spectrometer, the P-skin enables a simple “touch-and-detect” workflow without complicated sample preparation or transfer.

Using methylene blue as a model analyte, the P-skin achieved a detection limit of 5×10^{-8} M with a hand-held Raman system and 1×10^{-13} M with confocal Raman microscopy. The device maintained reliable SERS performance under bending, twisting, stretching, variable contact pressure, and repeated fabrication, demonstrating its mechanical robustness and signal reproducibility. We further developed a wet-touch strategy to recover residues from dried porous substrates, showing that substrate porosity, surface roughness, and water retention strongly influence contact-based molecular transfer. Finally, we demonstrated practical pesticide sensing by detecting thiram residues on paper, apple, avocado, and carrot surfaces, with a detection limit approximately 30 times lower than the U.S. EPA maximum residue limit.

This work establishes a skin-like, finger-wearable SERS interface for rapid field chemical identification, with potential applications in food safety, environmental monitoring, and precision agriculture.

Biography

Dr Yan Lu received his PhD from Monash University in 2023 and is currently a postdoctoral researcher in the Department of Biomedical Engineering at the University of Sydney. His research focuses on the controlled synthesis, assembly, and interface engineering of nanomaterials for wearable plasmonic sensors and flexible bioelectronics. By developing multifunctional nanomaterial-based platforms, his work addresses key challenges in conformal biointegration, stable signal transduction, and material functionality for practical wearable biosensing. His research provides material-level solutions for connected healthcare, smart medicine, soft robotics, and human–machine interfaces.

LASERS FOR LASERS: RAMAN SPECTROSCOPY OF LASER-INDUCED GRAPHENE FABRICATION

Sophie Cottam

[1]*School of Biomedical Engineering, University of Sydney*
[2] *School of Physics, University of Sydney*
[3] *Sydney Nano Institute, University of Sydney*
[4] *Charles Perkins Centre, University of Sydney.*

Laser-induced graphene (LIG) is becoming an increasingly popular method for the rapid, dry fabrication of conductive electrodes. Through the direct conversion of a polymer surface into graphene-like carbon, LIG enables the production of custom electrode designs without the need for complex manufacturing processes or wet chemical treatments. When combined with plasma functionalisation, LIG surfaces can be modified to facilitate the covalent attachment of biomolecules, expanding the potential applications of the technique in biosensing and cell culture platform fabrication.

To achieve consistent performance and scalable manufacturing of LIG-based devices, it is essential to develop a strong understanding of the relationship between fabrication parameters and material properties. Manufacturing parameters such as laser power, scanning speed, and substrate composition can significantly influence the structure, conductivity, and surface functionality of the patterned electrodes. As a result, reliable characterisation techniques are required to monitor and optimise the multi-step process.

Raman spectroscopy is a powerful analytical tool for the characterisation of LIG materials. Analysis of Raman spectra provides valuable insights into graphitisation, defect density, and structural changes introduced during both laser processing and plasma functionalisation. This presentation will provide an overview of the role of Raman spectroscopy in the optimisation of LIG electrode fabrication, highlighting how Raman-based characterisation can be used to guide process development.

Biography

Sophie Cottam is a final year PhD student in the Applied Plasma Physics and Surface Engineering group lead by Professor Marcela Bilek. Her research focuses on the use of dry synthesis methods for fabrication of advanced cell culture and biosensing platforms.

AN IN-DEPTH ANALYSIS OF ANCIENT EGYPTIAN CARTONNAGE USING OPTICAL PHOTOTHERMAL IR (O-PTIR) SPECTROSCOPY

Ali Ibrahim[1] and Dr Elizabeth Carter[2]

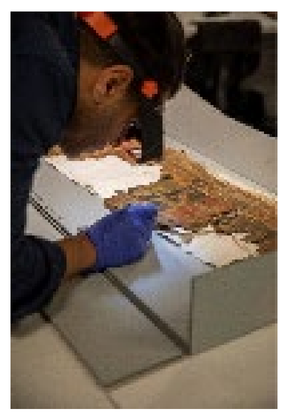
Chau Chak Wing Museum, The University of Sydney, Sydney, NSW, Australia.
Sydney Analytical, The University of Sydney, Sydney, NSW, Australia.

The talk will explore the application of a new technology called optical photothermal infrared (O-PTIR) spectroscopy. O-PTIR spectroscopy enables non-invasive analysis of organic and inorganic materials at the submicron scale. Complex sample preparation is not required, and the technique allows simultaneous collection of infrared and Raman data. To demonstrate the capabilities of the instrument, it has been applied to the analysis of an ancient Egyptian cartonnage, a late-period funerary artifact traditionally made from layers of linen or papyrus and adorned with intricate decorations. The primary focus is characterising the pigment composition and preparation layers used in these historical objects, providing deeper understanding of their artistic and cultural significance.

Key findings include the use of mixed materials in black pigments, indicating traditional methods of pigment preparation. The identification of animal glue in the red pigment, underscores the use of organic binders, standard practice in the late period of cartonnage production. The high spatial resolution of O-PTIR spectroscopy enables precise targeting of specific areas within complex mixtures and allows for identification of pigment signatures such as hematite and azurite. Analysis of the preparation layer revealed the presence of lipids, highlighting their role in enhancing the adherence and qualities of the preparation layer.

This work demonstrates O-PTIR spectroscopy as a powerful, non-invasive method for characterising complex cultural artifacts, enabling vital contributions to heritage conservation and restoration practices. The findings provide a foundation for further comparative studies, facilitating a better understanding of the materials and techniques employed in ancient artistic practices.

Biography



Ali Ibrahim is an archaeological and museum collections conservator specialising in the conservation of ancient materials. Since 2009, he has been working in the conservation and preservation of cultural materials. With a Bachelor's in Archaeology and a Master's in Museum Studies and management, he has worked extensively in Egypt and Chile across archaeological sites, museums, and cultural institutions, including roles at the Grand Egyptian Museum and the Giza Pyramids. Currently working at the Chau Chak Wing Museum, Ali focuses on artifact assessment, research, and community engagement, collaborating on projects that enhance public understanding of archaeological heritage.

SESSION 3 - VS FACILITY TOUR

SESSION 4 - LIFE SCIENCES

LIVE CELL IMAGING USING TIME-LAPSE FTIR SPECTROSCOPY

Ross M. Graham

School of Diagnostic & Molecular Sciences and Curtin Medical Research Institute, Curtin University, Western Australia

Synchrotron FTIR live cell imaging is a powerful technique that allows interrogation of biochemical changes in single cells following challenge. It allows analysis of cellular functions in their native environment, is non-destructive and does not require molecular labelling. However, like all techniques, it is not without its limitations. From a physiological viewpoint, mammalian cells do not exist in isolation and are responsive to signals from adjacent or distal cells. From a spectroscopic viewpoint, water absorbs in the infra-red region, and cells contain, and exist in, an aqueous environment.

As a model to investigate lipid dysregulation present in fatty liver, we incubated a mouse hepatocyte cell line with iron, a metal often present in excess in fatty liver. Cells were seeded on to CaF2 windows and sealed, along with experimental medium, in a modified Bioptechs flow cell available at the Australian Synchrotron's Mid-IR beamline. In each experiment, a single cell was chosen and mapped hourly for up to 8 hours. Spectra were collected in transmission mode using an 8.3 μm diameter aperture and a 3 μm step size.

Increases in the absorbance of the ester carbonyl band were consistent with an increase in esters (mainly triglycerides) present in iron-loaded cells compared to controls, as well as a rise in the triglyceride concentration over time under both conditions. Using the ratio of methylene to methyl absorbance as a measure of relative lipid chain length, chain length shortened over time in control cells, whereas it lengthened in iron-loaded cells. A pronounced increase in the absorbance of the olefinic band indicated an increase in total lipid unsaturation in iron-loaded cells. Analysis of the second derivative spectrum revealed a shift to higher wavenumbers, consistent with a shift to more poly-unsaturated lipids in the iron-loaded cells.

Synchrotron FTIR imaging is capable of deciphering biochemical processes in live cells over a period of at least 8 hours at sub-cellular resolution. Use of this technique has provided direct evidence of iron-associated lipid accumulation that may lead to hepatic steatosis in whole liver.

Biography

Dr Ross Graham is a Senior Lecturer in Genetics at Curtin University in WA where he leads a small research group that uses infra-red and X-ray fluorescence techniques to investigate the interaction between metals and lipids in the gastrointestinal system, including liver and pancreas.

Ross completed his PhD at the University of Western Australia then moved to London where he worked on the cobalt-containing vitamin, B12 (cobalamin). Upon return to Perth, he continued his work on biometals at Fremantle Hospital, investigating the link between hepatic iron and cholesterol. Now at Curtin University, he leads a small team using a multi-modal approach of synchrotron IR and XRF paired with molecular biology and traditional biochemistry to understand biometal- and lipid-associated mechanisms of disease.

NEAR INFRARED SPECTROSCOPY OF TWO HIGHLY CORRELATED CONSTITUENTS IN WHEAT GRAINS

Graeme D. Batten

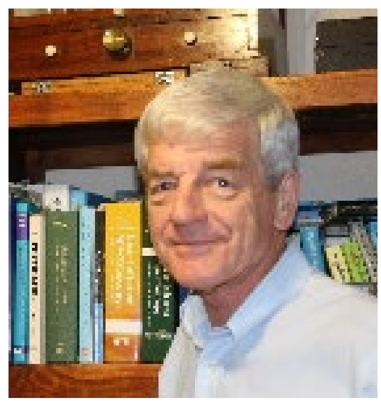
School of Life and Environmental Sciences, The University of Sydney, Sydney, NSW, Australia.

Australian wheat producers apply phosphate (P) fertilizer to achieve higher yields. Applying P increases the concentration of total-P in the grain (%P) and at the same time increases the proportion of this P 'stored' in an anti-nutrient compound called phytate. Reduced total-%P and phytate-bound-%P are desired for economic and health reasons.

The total-%P in wheats that achieve high yields could be reduced by 25-30%. Mutant genotypes and cultivars of cereals are available that have typical total-%P but phytate-bound-%P reduced by 50%. To make progress, plant breeders need a user-friendly analysis for each of these traits.

We are applying NIRS to identify wheat genotypes with a lower grain total-%P and also lower phytate-bound-%P; fully aware that total-%P and phytate-bound-%P are usually highly correlated. This is not ideal for NIRS analyses. I will present a progress report.

Biography



Graeme has a Master's Degree in Rural Science from the University of New England and a PhD in Science (Botany) from the Australian National University. From 1970 to 2000 he was with NSW Agriculture (NSW DPI) researching the fertilizer requirements of crops and pastures in Southern NSW. In the late 1980's he applied near infrared spectroscopy (NIRS) to improve the utilization of nitrogen in rice and wheat crops. From 2000-2005 he was Professor of Irrigation at Charles Sturt University. Graeme has been an editor of the Journal of Near Infrared Spectroscopy since 1994, serving as Editor-in-Chief from 2004 to 2017. As an Honorary Professor he continues to apply NIRS to enhance food security.

RAPID BIOCHEMICAL PROFILING OF PROBIOTIC EVS USING HIGH-THROUGHPUT FTIR SPECTROSCOPY

Luke Pevey

Sydney Pharmacy School, The University of Sydney, Sydney, NSW, Australia.

The successful clinical translation of extracellular vesicle (EV) therapeutics depends on biomanufacturing processes that consistently meet defined critical quality attributes (CQAs). This requires rapid, reliable, and scalable analytical methods capable of assessing compositional features central to EV function. Conventional assays are slow, costly, and labour-intensive, limiting their suitability for routine monitoring and batch release. Vibrational spectroscopy offers a promising alternative if adapted into an efficient high-throughput workflow.

We developed a high-throughput FTIR platform for biochemical profiling of EVs using the Bruker TENSOR HTS-XT system. The method enables rapid, non-destructive, label-free assessment of EV composition. A custom Python-based pipeline generates biochemical heatmaps that quantify lipid, protein, nucleic acid, and carbohydrate signatures, providing detailed compositional fingerprints and supporting batch-consistency evaluation. This framework establishes a foundation for future AI-driven analytical tools capable of real-time batch classification and process-deviation detection, ultimately enabling more precise and cost-effective EV biomanufacturing.

Biography

Luke Pevey is a PhD candidate in the Sydney Pharmacy School at the University of Sydney. His research focuses on establishing a robust biomanufacturing and bioprocessing pipeline for postbiotics, with particular emphasis on probiotic-derived biologicals such as cytoplasmic membrane vesicles (CMVs) and outer membrane vesicles (OMVs). His work integrates bacterial fermentation, downstream processing, and high-throughput vibrational spectroscopy to develop reproducible, scalable methods for analysing postbiotic products, supported by Python-based statistical and visual analytics. Luke's broader research interests include bioprocess optimisation, spectral informatics, and the application of chemometric tools to enhance quality control in complex biological systems.

SESSION 5 - LIFE SCIENCES

ASSESSMENT OF LATE POSTMORTEM INTERVAL OF SKELETAL REMAINS USING RAMAN AND FTIR SPECTROSCOPY

Hayley Green

School of Science, Western Sydney University, NSW, Australia.

The estimation of postmortem interval (PMI), especially the late PMI when remains are 31keletonized, is an important and challenging task in forensic investigations. In spite of this, there is still a lack of effective means to perform an accurate and reliable late PMI estimation.

Studies assessing the application of vibrational spectroscopy, including Fourier Transform Infrared (FTIR) and Raman spectroscopy for the forensic investigation of postmortem changes to bone have gained momentum recently. However, no two methodological approaches are the same, and while results demonstrate vibrational spectroscopy has "potential" in estimating PMI from skeletal remains, currently published methods are not yet case-work ready. This presentation will detail pilot results of two studies assessing the use of benchtop and field portable vibrational spectroscopic methods (Raman and FTIR) to estimate PMI of unburied skeletal remains. Issues, limitations and future directions will also be discussed.

Biography

Dr Hayley Green is a Forensic Anthropologist and Senior Lecturer in the School of Science at Western Sydney University. Hayley collaborates with the Australian Facility for Taphonomic Experimental Research (AFTER) at University of Technology Sydney to develop time since death methods which are applicable to the specific characteristics an Australian climate, studying how bodies decompose in different microclimates and the resultant weathering patterns that can be seen on bones.

She is also investigating the use of multidisciplinary techniques, including benchtop and field portable vibrational spectroscopic methods, to identify potential chemical signatures in bone samples in a non-invasive manner to improve casework capabilities in the estimation of time since death of skeletal remains. As well as observing physical changes to the body as it decomposes, Dr Green undertakes multidisciplinary research with collaborators in the School of Science and the Advanced Materials Characterisation Facility (AMCF) to investigate the impact of the environment on decomposition and in turn, how the body leaves it mark on the environment.

SERS-BASED PLASMONIC BIOSENSOR FOR 3D CARDIAC MODEL METABOLITES MONITORING

Xiaorui Cao

The University of Sydney, Sydney, NSW, Australia.

Local pH is an important indicator of cardiac cell metabolism, ion homeostasis and contractile function. Abnormal pH regulation can accompany metabolic stress, impaired cellular function and drug-induced cardiac injury. Monitoring pH in three-dimensional cardiac spheroids is therefore valuable for understanding how biochemical changes develop within cardiac tissue models and how these changes relate to functional responses.

Unlike conventional two-dimensional cultures, cardiac spheroids possess a complex three-dimensional structure in which nutrient transport, oxygen availability and cellular metabolism can vary between the surface and the core. As a result, pH may be spatially heterogeneous and change dynamically over time. Conventional single-point measurements cannot capture these local variations and may therefore overlook important biochemical information within the spheroid.

Here, we apply surface-enhanced Raman spectroscopy (SERS)-active microsensors for spatiotemporal pH monitoring in intact cardiac spheroids. The microsensors are incorporated throughout the spheroid, enabling Raman mapping of local pH distributions and repeated measurements over time. The platform is used to study size-dependent pH heterogeneity and pH changes associated with doxorubicin-induced cardiotoxicity.

By providing both spatial and temporal information, this approach moves beyond conventional point-based pH measurements and enables biochemical changes to be correlated with cardiac contractile behaviour. It offers a promising platform for studying cardiac physiology, tissue heterogeneity and drug-induced injury in three-dimensional in vitro models.

Biography

Xiaorui Cao is a PhD candidate at the University of Sydney under the supervision of Professor Wenlong Cheng. She completed her previous degree at Monash University and joined the Cheng Nanobionics Research Laboratory. The group conducts interdisciplinary research across nanomaterials, electronics and biology, with a focus on plasmonic nanostructures, biosensing and adaptive sensing technologies. Within this research environment, Xiaorui develops surface-enhanced Raman spectroscopy (SERS)-based biosensors for chemical detection and for monitoring biochemical changes in three-dimensional biological models. Her current work focuses on spatial pH monitoring in cardiac spheroids, with potential applications in cardiotoxicity assessment and drug screening.

LOW-WAVENUMBER CHARACTERISATION OF MULTI SUBSTITUTED APATITES

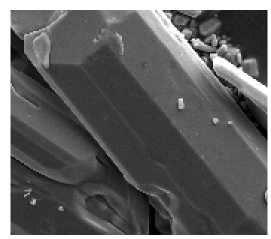
Cameron A. Isaacs, Claire E. Lenehan, Sara J. Fraser-Milller

College of Science and Engineering, Flinders University, Bedford Park, South Australia 5042, Australia

Multi substituted apatites are the major inorganic component of teeth and bone and in addition invasive calcium deposits known as microcalcificaitons.[1] These microcalcifications often appear colocalised with diseases such as cancer and literature shows that the crystallinity and substitution of these apatites can be an indication of disease state.[2] Unfortunately, the most common ways to detect microcalcificaitons are X-Ray imaging techniques that cannot resolve the chemical and mineralogical information needed for diagnosis without a subsequent biopsy. Compounding to this, quite incredibly, only around 20% of biopsies return a positive diagnosis, giving justification for some sort of technique that can rapidly reveal the key metrics needed for diagnosis.

Apatites are simply the most common mineral form of calcium phosphate with the formula (Ca5(PO4)3X) where X is commonly Cl-, F- or OH- and as such they can be straightforwardly characterised by techniques such as X-Ray diffraction and vibrational spectroscopy.[3] Low-Wavenumber techniques in particular, that probe lattice modes dictated by crystal structure and long range order, that often occur at Raman shifts <300 cm-1 are particularly sensitive to both changes in crystallinity and substitution. In this work a range of apatites substituted with varying amounts of Na^{+}, Mg^{2+} and CO_3^{2-} were synthesised, dictated by a design of experiments approach. Standard X-Ray diffraction and vibrational spectroscopy techniques were utilised alongside low-wavenumber Raman to compare and contrast their ability to resolve information on crystallinity and substitution. Low-Wavenumber Raman was particularly sensitive to cationic substitutions which are often difficult to observe in the fingerprint region, establishing it as at least a complementary technique within this sort of application.

Biography



Mr. Cameron Isaacs is a second-year PhD candidate at Flinders University who's research focuses on using low-wavenumber spectroscopy to examine the long-range order of minerals and similar materials such as MOF's. Cameron spent his honors year designing a portable fluorescence detector with a simple LED, polarizing films, a long pass filter and a photodiode that was able to detect fluorescently labelled proteins down to levels competitive with benchtop units. Cameron is an expert user of free space spectroscopic techniques and has developed programs that enable low-frequency Raman mapping on a free space laser system of samples as small as 100 microns. Cameron also utilizes his multivariate statistical skills to analyze cultural ochre samples in an attempt to understand the effects that heating may have on their mineralogy.

1. Evans, A. J., A. R. M. Wilson, H. C. Burrell, I. O. Ellis, and S. E. Pinder. 1999. 'Mammographic features of ductal carcinoma <in situ (DCIS) present on previous mammography', Clinical Radiology, 54: 644-46.
2. Baker, R., K. D. Rogers, N. Shepherd, and N. Stone. 2010. 'New relationships between breast microcalcifications and cancer', Br J Cancer, 103: 1034-9.
3. Kirkham, Joshua, Timothy M. Korter, Kārlis Bērziņš, Cushla M. McGoverin, Keith C. Gordon, and Sara J. Fraser-Miller. 2023. 'Characterization of Variably Substituted Hydroxyapatites Using Low-Frequency Raman Spectroscopy', Crystal growth & design, 23: 5748-61.

SESSION 6 - ENVIRONMENT

FROM TERRASPEC TO PREDICTIVE MINERAL INTELLIGENCE: QUANTIFYING INFRARED SPECTROSCOPY FOR MINING

Thomas Rodemann

Central Science Laboratory, University of Tasmania

Near-infrared (NIR) spectroscopy has been widely used in mineral exploration and mining for more than three decades, most notably through SWIR instruments such as *TerraSpec*. These tools transformed exploration by enabling rapid, non-destructive identification of alteration minerals in the field and core shed. Yet despite their widespread adoption, the way NIR data were used changed remarkably little over time. Outputs remained largely qualitative or semi-quantitative, relied on expert interpretation, and provided indirect proxies for mineral chemistry. Quantitative mineralogy and geochemistry continued to depend on slow, destructive, and expensive laboratory methods such as XRD and ICP-MS.

This talk examines why NIR spectroscopy in mining plateaued technologically, despite major advances in instrumentation and data acquisition. The key limitation was not hardware, but the absence of validated mineral–spectral–chemistry libraries and predictive models capable of converting infrared spectra into quantitative, decision-ready information. I will then describe how research at the University of Tasmania's Central Science Laboratory (CSL) and Centre for Ore Deposit and Earth Sciences (CODES) has overcome this bottleneck. By coupling high-resolution FT-NIR and FT-IR spectroscopy with a world-leading mineral and mineral-chemistry database, we have developed predictive infrared models that deliver quantitative mineral proportions and mineral chemistry directly from spectral measurements.

These advances are now translated through ScopeIR, a UTAS spin-out company delivering integrated field and laboratory IR platforms with automated cloud analytics. ScopeIR transforms infrared spectroscopy from a specialist, interpretive technique into a scalable quantitative measurement system, validated against laboratory standards and deployed with major mining companies. The trajectory from TerraSpec to ScopeIR highlights how vibrational spectroscopy, when combined with domain-specific datasets and predictive modelling, can fundamentally reshape exploration, orebody knowledge, and mining efficiency.

Biography

A/Prof Thomas Rodemann is a vibrational spectroscopist with more than two decades of research experience spanning the development and application of infrared and Raman techniques across science and industry. He is Director of the Central Science Laboratory and Principal Research Fellow in Vibrational Spectroscopy at the University of Tasmania, and since 2024 has served as Technical Lead of ScopeIR, a UTAS spin-out company advancing quantitative infrared methods for the resources sector.

Trained as a chemist, he has built an interdisciplinary career applying micro-Raman, FT-IR, and NIR spectroscopy across geoscience, environmental monitoring, agriculture, and marine science. His work consistently focuses on extracting quantitative, decision-ready information from complex spectral datasets, bridging the gap between analytical capability and operational use. Over more than twenty years, his research has been supported by major national and industry partners, including the Australian Research Council, AMIRA Global, Wine Australia, and Newcrest Mining, leading to innovations in rapid spectroscopic imaging, mineral systems analysis, and environmental microplastic detection.

Through his role with ScopeIR, A/Prof Rodemann contributes to the maturation of predictive infrared spectroscopy from a specialist analytical approach into a scalable, industry-validated measurement capability.

SPATIAL DIFFERENCES IN AGGREGATE STABILISED MINERAL ASSOCIATED ORGANIC MATTER UNDER THREE AGRICULTURAL SOILS

Rachel Yamamoto

The University of Sydney, Sydney, NSW, Australia

Soil organic matter (SOM) dynamics are shaped by both inputs, often originating from plants and their roots, and their interactions with soil minerals and the microbial activity of the soil. Yet SOM stability is negatively affected by external anthropogenic activities such as land clearing and management. The preservation and longevity of SOM has been attributed to associations with clay minerals, referred to as mineral-associated organic matter (MAOM). MAOM prevents microbial decomposition and slows turnover via two co-occurring processes; mineral adsorption and physical occlusion through aggregate formation. The mineralogy, surface chemistry and clay mineral content of the soil can greatly determine the type of bonding, the strength of SOM bonding, and the quality of the retained SOM.

However, common bulk soil measurements mean that the diversity of SOM qualities are lost when structural and chemical differences in organic matter and clay minerals occur on a spatial scale of micro- to nano-metres. In this study, we used OPTIR and synchrotron based FTIR microspectroscopy on microaggregates collected from three soils under ryegrass or clover to resolve differences in the organo-mineral interactions between agricultural soils at a nanometre scale. Dried water-stable aggregates were sliced and analysed in the mIRage in co-propagation mode using the 532 nm laser. Hyperspectral scans were collected and organic bands corresponding to carboxylates, amide I, amide II, aliphatic, phenol and combined carboxylate-amide were selected, and mineral bands for Si-O, Si-O-Si, Si-O-Al, Al-O and Fe-O bonds selected for analysis.

SOM appeared strongly co-located with each other and to occur in hotspots with high surface irregularities where SOM remained protected. Our results shed light on how different crop species influence rhizodeposition and root morphology, and those interactions with the soil geochemistry affects the stabilisation and quality of SOM in MAOM fractions.

Biography

Rachel Yamamoto completed her honours at USYD in soil microbial physiology, before working as a research associate with Professor Balwant Singh for almost 2 years on a DAFF Soil Science Challenge project. The project aimed to disentangle the key drivers involving the plant-soil-microbe nexus that both preserves and mineralises organic carbon in agricultural soils across NSW. Part of this project included analysing soil aggregates with the mIRage at Sydney Analytical as well as using synchrotron-based FTIR microspectroscopy and a suite of other IR and mass-spectrometry analyses. Rachel is currently doing a PhD at USYD with Professor Charles Warren on soil microbial ecology, nutrient availability and competition.

ASSESSING FOCUS ACCURACY AND SUBSTRATE EFFECTS IN FPA-BASED MICROPLASTIC ANALYSIS COMPARING LUMOS II AND SPERO SYSTEMS

Christine Fink[1], Elizabeth A. Carter[2,3], Abbas El-Zein[1]

[1]School of Civil Engineering, The University of Sydney, Sydney, NSW, Australia.
[2] Sydney Analytical, The University of Sydney, Sydney, NSW, Australia.
[3] School of Chemistry, The University of Sydney, Sydney, NSW, Australia.

Accurate detection of environmental microplastics depends strongly on substrate selection and precise optical focusing, particularly when using focal plane array (FPA)-based infrared microscopy. This study compares the performance of the LUMOS II system for analysing environmental microplastic samples filtered onto Anodisc versus silicon substrates, while assessing how focus quality influences particle detection and quantification.

Anodisc substrates, although commonly used for microplastic filtration, present significant focusing challenges due to their opaque, highly textured aluminium oxide surface. This leads to reduced infrared image clarity, inconsistent spectral quality, and an increased risk of particle undercounting when the focal plane does not coincide with the particle surface. In contrast, silicon filters provide a smooth and reflective substrate that potentially supports more stable focusing conditions and improved spectral quality. Full-filter FPA mapping is acquired as a multi-tiled dataset fixed at the focal plane determined at the start of measurement. As a result, surface height variations and uneven topography of Anodisc substrates amplify defocus artefacts and degrade detection performance.

Comparisons with the SPERO chemical imaging infrared microscope further highlight methodological trade-offs. The SPERO system enables substantially faster acquisition, enabling high-throughput screening of environmental samples, but at the expense of a smaller spectral range and reduced spectral resolution. Subsequent processing of both datasets using microparticleAI will allow evaluation of potential differences between SPERO and LUMOS II data, providing insight into how variations in spectral quality may influence the detection of microplastics.

Overall, these results demonstrate that filter material, surface characteristics, and optical focus are critical determinants of detection reliability in FPA-based infrared microplastic analysis. Methodological choice, particularly regarding instrument speed, spectral quality, and substrate selection, must therefore be carefully balanced to minimise systematic underestimation in environmental monitoring.

Biography

Christine Fink is a PhD student at the University of Sydney, Australia, where her research focuses on developing innovative spectroscopic techniques for the characterisation of nanoplastics. She works as a technical officer at Sydney Analytical.

Christine holds both a Bachelor's and Master's degree in Biotechnology. She also participated in the six-week HE578 research cruise as part of the "FACTS – Fluxes and Fate of Microplastics in Northern European Waters" project, investigating the distribution of microplastics throughout the Atlantic Ocean water column. Her work integrates biotechnology, environmental science, and advanced spectroscopic methods, with a strong focus on the detection of micro- and nanoplastics.

ENVIRONMENTAL PARTICLES DETECTION BY QCL IR IMAGING AND NEMS-FTIR SPECTROSCOPY

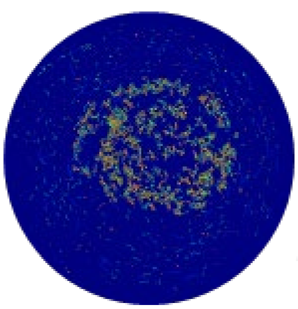
K.M. Koman Tam[1], David Marston[1], Dan Wu[2], Domenic Dreisbach[2]

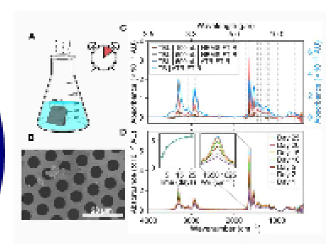
[1]Bruker Pty Ltd, 1/28A Albert Street, Preston VIC, 3072, Australia.
[2]Bruker Optics GmbH & Co. KG, Rudolf-Plank Straße 27 · 76275 Ettlingen, Germany.

Vibrational spectroscopy (FTIR and Raman) is a key analytical technique in polymer research, manufacturing and recovering business. The breakdown of the plastics into micro-and-nano-plastics has gained strong awareness with regulatory requirements and ISO standards currently in place. With advanced technology in quantum cascade laser (QCL) FTIR and powerful machine- and deep-learning classification tools, micro/nanoplastics classification, counts and shapes can be rapidly analysed and can be used for high throughput routine commercial testing lab analysis.

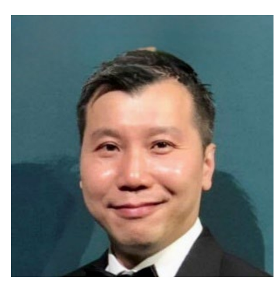
1/ Microplastics classification by QCL FT-IR microscopy:
FPA offers full spectral range information, but measurement time could still be hours and even longer for single element detector. A complete QCL MP analysis with machine and deep learning classification on the whole 25mm filter takes less than 30 minutes (approx. 23 million spectra) with classification, shape and counts.

2/ New EMILIE™ nanoelectromechanical systems (NEMS) with Fourier transform infrared accessories for nano plastics/aerosol detection and polymer characterisation.
While Raman and O-PTIR microscopes are the current go-to method for nanoplastics, but instrumentation is a significant investment. The new EMILIE™ NEMS-FTIR accessory offer relatively low cost on existing FTIR system, cryogen-free detector with low intrinsic noise, independent by spectral range, resilient to optical artefacts by conventional microscopic techniques. EMILIE™ enables the bulk chemical characterisation of nanomaterials, including ultrafine aerosols, nanoplastics, biopharmaceuticals and nanomedicines, with a sensitivity reaching picograms levels, while samples can be directly collected from powders, aerosols, dispersions or solutions.





Biography



Dr Koman Tam completed his PhD in 2006 at the Vibrational Spectroscopy Facility (now Sydney Analytical) at The University of Sydney. His research focused on developing non-destructive methods for breast cancer diagnosis using infrared (IR) and Raman spectroscopy. He worked under the supervision of Prof. Peter Lay, the late Assoc. Prof. Bob Armstrong, and Dr Liz Carter. His PhD work mainly involved sample preparation and imaging techniques to classify cancer using statistical analysis. In 2007, he joined Bruker as an Applications and Product Specialist. Since then, he has worked on infrared and Raman microscope technologies for both academic and industrial use, including applications in materials science, biospectroscopy, and micro- and nanoplastics analysis.

FROM ONE SOIL SPECTRUM TO MULTIPLE ENVIRONMENTAL INFORMATION: MID-INFRARED SPECTROSCOPY FOR SOIL BIOLOGY, CARBON, AND MICROPLASTICS

Kim Tran

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Healthy soils are essential for sustainable food production, biodiversity, and climate resilience, yet comprehensive soil assessment remains time-consuming and costly because multiple laboratory analyses are often required. Mid-infrared (MIR) spectroscopy offers a rapid, non-destructive alternative capable of simultaneously providing information on a range of soil properties.

Our research demonstrates the potential of MIR spectroscopy, combined with chemometric and machine-learning approaches, to rapidly predict soil microbial properties and soil carbon fractions across diverse Australian soils. Models developed from high-throughput spectral measurements showed promising performance for key biological and carbon indicators. In addition, laboratory studies using microplastic-spiked soils highlight the potential for MIR spectroscopy to detect selected microplastic types and concentrations, providing an important proof-of-concept for future environmental applications. The studies further demonstrate the influence of soil texture and other soil characteristics on prediction accuracy and emphasise the importance of robust calibration strategies.

MIR spectroscopy can extract multiple layers of information from a single spectral measurement, and thus has the potential to transform soil monitoring into a rapid, scalable, and cost-effective approach. This framework supports environmental monitoring, digital agriculture, and nature-positive land management by providing timely information on soil biology, carbon dynamics, and contaminant status.

Biography

Dr Kim Tran is a Postdoctoral Researcher at the Sydney Institute of Agriculture and the School of Life and Environmental Sciences, the University of Sydney. Her research focuses on emerging contaminants, environmental monitoring, and soil health, with expertise spanning ecotoxicology, microplastics, soil carbon, and environmental monitoring. She applies vibrational spectroscopy and machine learning to develop rapid, high-throughput approaches for assessing soil properties and emerging contaminants. Her interdisciplinary research aims to support evidence-based environmental management and nature-positive agricultural systems.

TOWARD RELIABLE MICROPLASTICS DATA: CHALLENGES IN SPECTROSCOPIC ANALYSIS AND MACHINE LEARNING.

Benedikt Hugnafl

Hufnagl Chemometrics GmbH

The analysis of microplastics in environmental samples using µFTIR imaging is widely applied, yet translating hyperspectral data into reliable and comparable results remains challenging. Environmental samples introduce strong variability through degradation, matrix effects, particle morphology, and physical phenomena such as scattering and absorption, all of which can obscure spectral signatures and complicate polymer identification.

While spectral library matching is commonly used, it is limited by incomplete reference coverage and sensitivity to measurement conditions. Machine learning approaches offer improved robustness, scalability, and processing speed, and are increasingly recognized in emerging standardization frameworks. However, they also introduce new challenges related to training data quality, domain shift, and model transferability across instruments and sample types.

This presentation discusses key analytical challenges in spectroscopic microplastics analysis and highlights how they affect data reliability and comparability. The goal is to provide a realistic perspective on current limitations and to underline the importance of transparent, validated, and standardized workflows for improving confidence in environmental microplastics assessments

Biography

Benedikt Hufnagl is a chemometrician and entrepreneur working at the intersection of machine learning and spectroscopic data analysis. He is the founder and CEO of Hufnagl Chemometrics GmbH, where he develops software tools that make advanced chemometric methods more accessible to researchers and practitioners. He is passionate about chemometrics as a discipline and strongly believes that powerful data analysis should be usable beyond specialist groups.

His work is driven by the goal of improving the quality and comparability of microplastics data, so that it can better support scientific understanding and environmental decision-making. In this context, he also contributes to international standardization efforts at ISO, focusing on how data quality and consistency can be improved across laboratories and workflows

SESSION 7 - ENVIRONMENT

NEXT GENERATION OF INSTRUMENTS REQUIRED - COMBINED AND CORRELATIVE SEM, EDS, XRM, CL, RAMAN AND OPTICAL SYSTEM (COLOUR-CL-GSR SYSTEM) FOR GUNSHOT RESIDUE AND MINERALOGICAL ANALYSIS

Richard Wuhrer

Advanced Materials Characterisation Facility, Western Sydney University.

Over the past 20 years it has become possible to analyse crushed mineral material, as well as gunshot residue (GSR) particles, using automated SEM and EDS systems. These processes are suitable for large-scale automatic analysis applications for both mineral liberation analysis (MLA) and GSR analysis. However, these techniques do not work well with minerals with low concentrations of light elements such as Li, Be and B, any water of hydration (.nH2O), in the case of GSR newly available heavy metal free (HMF) cartridge primers (organic primers).

Consequently, a new, rapid method of materials analysis, as well as mineral and inorganic particle classification, has been explored using a combination (hybrid system or toolbox) of well-established techniques such as optical microscopy, SEM, EDS, Raman spectroscopy, Cathodoluminescence (CL) and Fluorescence [1, 2]. The SEM and optical systems allow the user to find particles of interest, the EDS to determine detectable elements, and the Raman to distinguish between polymorphs to ratify non-detectable elements. GSR of particles and/or X-Ray mapping (XRM) of materials and particles, allows for mapping of chemical/elemental information, and hence chemical phase mapping (CPM) [3].

The presentation will discuss the development and incorporation of new instrumentation on a traditional large scale SEM and Phenom desktop SEM that will benefit and assist analysis for many applications, and will cover the next generation of instrumentation required for those applications.

Biography

Dr Richard Wuhrer is the Facility Research Manager of the Advanced Materials Characterisation Facility (AMCF) at Western Sydney University (WSU) and holds a PhD in Applied Science from UTS. Richard has extensive experience on various scanning electron microscopes, microanalysis systems, X-ray mapping and X-ray diffraction systems. He has been involved in major research activities in the field of characterisation techniques, SEM/ESEM, thermal analysis, vibrational spectroscopy and X-Ray Diffraction (XRD). He has also taught many courses and workshops on these techniques, as well as in the field of Materials Science and Engineering (Metallurgy, Organic and Inorganic Materials, Corrosion Science, Composites and Surface Engineering). He has extensive experience and successful collaborations with industry and instrument manufacturers in these areas.

Richard is a former President of the Australian Microbeam Analysis Society (AMAS). He has over 250 reviewed publications on a variety of topics from art works to gunshot residue analysis, surface engineering, biomimicry, development of new alloys and new materials. His main-focus however, remains on characterisation techniques and further development of these techniques through combining systems and aiding in the analysis of materials and biological materials.

MULTIMODAL HIGH-SPEED LASER-SCANNING SUBMICRON INFRARED (O-PTIR) AND STIMULATED RAMAN (PT-SRS) PLATFORM FOR REAL-TIME LABEL-FREE CHEMICAL IMAGING

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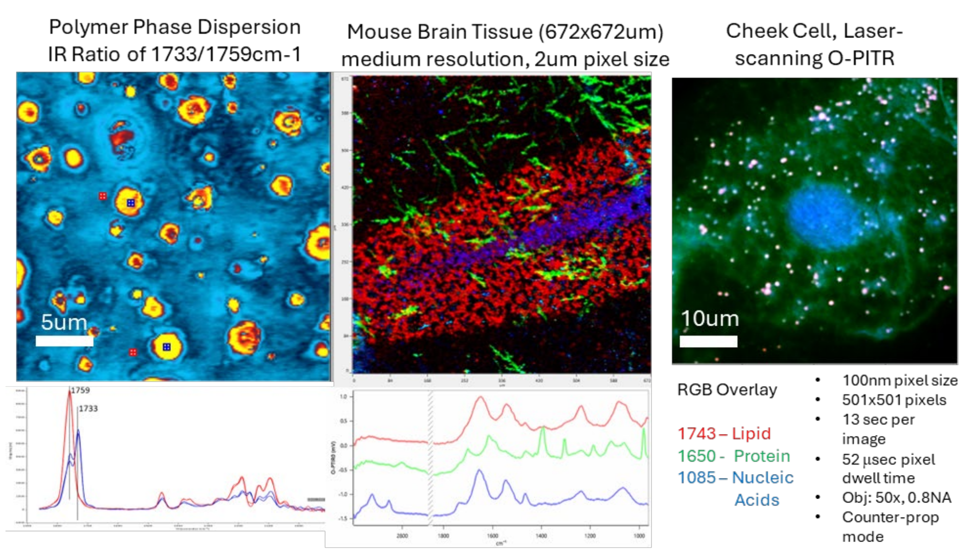
We describe a new laser-scanning microscope developed for real-time, label-free vibrational chemical imaging, integrating Optical Photothermal Infrared (O-PTIR) and Photothermal Stimulated Raman Scattering (PT-SRS) also known as Stimulated Raman Photothermal (SRP), modalities into a single multimodal, correlative platform. These techniques were originally developed in the laboratory of Prof. Ji-Xin Cheng at Boston University, whose group also contributed valuable collaboration during the development of the current commercial system.*

The platform enables true sub-micron spatial resolution and high-speed chemical imaging across a range of biological and materials science applications. High-speed synchronized IR and probe beam laser scanning supports efficient large-area imaging, with full hyperspectral data cubes acquired in minutes. The system also supports three-dimensional depth-resolved chemical imaging. To accommodate a broad range of sample types, the instrument supports both co-propagating and counter-propagating beam geometries, enabling measurements on IR-transparent and IR-opaque substrates. The combination of OPTIR and PT-SRS provides complementary vibrational contrast within one system, enhancing chemical specificity and enabling broader applicability to complex samples. The platform also includes multi-line widefield and laser-scanning confocal fluorescence, enabling fluorescence-guided infrared and Raman measurements. This facilitates correlative imaging in cellular biology, pathology, and functional materials research. We will present representative datasets from O-PTIR and PT-SRS imaging, including mixed polymer standards, subcellular structures (e.g., lipid dynamics in live cells), brain tissue sections, and microplastic mapping. These examples demonstrate the system's ability to support both high-resolution imaging and efficient analysis over extended areas.



ADVANCED INSTRUMENTS FOR RESEARCH, SAFETY AND SECURITY

Derek Huxley

Warsash Scientific

Advances in optical spectroscopy and field-deployable analytical technologies are transforming the way researchers, first responders, law-enforcement agencies, customs officers and industrial users identify, characterise and monitor materials. This presentation highlights recent advances in Raman and near-infrared (NIR) spectroscopy for research, safety, security and field-based chemical identification. Attendees will gain an overview of the latest capabilities from Renishaw Raman spectroscopy, including the inVia research-grade Raman microscope, Virsa Raman analyser, advanced chemical imaging and live focus-tracking technologies.

The talk will also review Thermo Scientific field instruments for rapid identification of narcotics, explosives, hazardous chemicals and unknown materials. In addition, emerging solutions from 908 Devices, including the NIRLab platform, a cloud-based NIR spectrometer for presumptive narcotics and materials identification, and Lightnovo portable Raman spectrometers will be discussed, demonstrating how modern spectroscopy is enabling faster decisions, improved safety outcomes and new opportunities for laboratory, field and point-of-care applications.

Biography

Derek Huxley is the Managing Director of Warsash Scientific and has more than 33 years of experience in the sales, application support and deployment of advanced molecular spectroscopy systems. His expertise spans research-grade and field-portable Raman, FTIR and near-infrared (NIR) spectroscopy, supporting applications in scientific research, materials characterisation, pharmaceuticals, forensics, hazardous materials identification, narcotics detection, and public safety.

Throughout his career, Derek has worked closely with universities, research institutes, industry and government agencies across Australia and New Zealand, as the product manager for Renishaw Raman Spectroscopy Products group, helping users apply spectroscopy solutions for both laboratory-based investigations and real-world field operations. He has a particular interest in the translation of Raman spectroscopy into practical tools for safety & security and presumptive narcotics identification across the Oceania region.

WORKSHOP - MicroparticlesAI

BEYOND SPECTRAL LIBRARIES: AI-ASSISTED MICROPLASTICS ANALYSIS WITH MICROPARTICLESAI

Benedikt Hufnagl

Hufnagl Chemometrics GmbH, Austria

The reliable detection and characterization of microplastics in complex samples requires robust and standardized analytical approaches. This workshop introduces the principles of chemometrics and machine learning in microplastics analysis, combined with a hands-on exploration of microparticlesAI, the first platform-independent software for μ(FT)IR hyperspectral imaging across multiple instrument vendors.

The first part covers key concepts in chemometrics, including the differences between spectral library search and machine learning models, strategies for building representative training datasets, and the role of iterative improvement and domain shift. Fundamental principles of model training and validation are discussed in the context of current standards, particularly ISO 24187:2023 and ISO 16094-2:2025.

The second part presents microparticlesAI and its application in real-world analysis. The software enables automated import, calibration, detection, and characterization of microplastics and microfibers from μ(FT)IR imaging data. Its machine learning models support a wide range of polymer types relevant to regulatory frameworks. Emphasis is placed on how the software's features address ISO requirements such as reproducibility, validation, and quality control. Participants will explore different application-specific models (e.g., environmental, food, textiles) and learn how matrix effects influence model performance.

Particle and fiber analysis is further illustrated through morphological descriptors such as Feret parameters, equivalent diameter, and fiber skeletonization, alongside the interpretation of classification quality scores. Strategies for handling large datasets, including filtering based on quality metrics, are also introduced.

In the practical session, participants will analyze real-world samples and explore challenges such as spectral ambiguity, expert bias, and the influence of total absorption and Mie scattering. They will create a test dataset for validation according to ISO 24187:2023 and compare machine learning model performance.

Overall, the workshop provides a compact, application-oriented introduction to AI-assisted microplastics analysis, combining theoretical foundations, standardization, and hands-on experience with a vendor-independent software platform.

Biography

Benedikt Hufnagl is a chemometrician and entrepreneur working at the intersection of machine learning and spectroscopic data analysis. He is the founder and CEO of Hufnagl Chemometrics GmbH, where he develops software tools that make advanced chemometric methods more accessible to researchers and practitioners. He is passionate about chemometrics as a discipline and strongly believes that powerful data analysis should be usable beyond specialist groups. His work is driven by the goal of improving the quality and comparability of microplastics data, so that it can better support scientific understanding and environmental decision-making. In this context, he also contributes to international standardization efforts at ISO, focusing on how data quality and consistency can be improved across laboratories and workflows.