November
12-13
2024

RamanFest
Paris | FRANCE

International Conference on
Advanced Applied Raman Spectroscopy

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# RamanFest
## November 12-13 2024
### Paris | FRANCE

## FOREWORD

On behalf of the Organising and Scientific Committees, we take great pleasure in welcoming you to Paris (France) for this new edition of the RamanFest International Conference (RamanFest2024).

The 11th International Conference on Advanced Applied Raman Spectroscopy (RamanFest2024) will feature presentations from world-leading Raman experts and researchers using the technique across varied applications within life science, materials science, and energy and environmental analysis. It will bring together the world's Raman community to share, learn and discuss how Raman spectroscopy is being applied to today's problems and pioneering tomorrow's capabilities.

We are indebted to HORIBA Scientific for their help and financial support. We also would like to thank all the speakers, partners, exhibitors and participants that joined us in person this year.

Hope to see you again in the next edition of RamanFest.

RamanFest2024 Organising Committee.

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# HORIBA

**HORIBA Scientific** (www.horiba.com) is proud to sponsor RamanFest 2024. HORIBA Scientific provides an extensive array of instruments and solutions for applications across a broad range of scientific R&D and QC applications.

Our proven quality and trusted performance can be found in over 500 types of scientific analyzers for Raman spectroscopy, fluorescence spectroscopy, atomic force microscopy, X-ray fluorescence spectroscopy, elemental analysis, GDOES, ICP-OES, particle characterization, forensics, spectroscopic ellipsometry, sulfur-in-oil, surface plasmon resonance imaging (SPRi), water quality measurements, custom spectroscopy solutions and OEM spectroscopy components.

Our instruments are found in universities, industries, research institutions, and government agencies. HORIBA provides multi-faceted data solutions in some of the most advanced science and technologies – assisting the most cutting-edge research in uncharted territories, and fueling applications in life sciences, pharmaceutical, materials research, food and agriculture, environmental, energy, water etc.

In 2019 HORIBA has celebrated the 200th anniversary of its optical spectroscopy roots. The Maison Soleil was founded in 1819 by Jean-Baptiste Soleil, becoming in 1923 the company Jobin Yvon through association with Amédée Jobin and Gustave Yvon. The technical foundation given by the Maison Soleil and the subsequent Jobin Yvon company remains at the heart of HORIBA's spectroscopy products, which are renowned for their performance and quality.

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Created through the business combination between the Keopsys and Quantel Groups in October 2017, **LUMIBIRD** is a mid-size firm with more than 1000 employees, revenues of over 191 M€, and offices in Europe, North America, China, Japan and Australia.

With 50 years of experience and expertise in 3 key technologies – solid-state lasers, laser diodes and fiber lasers – the group designs, manufactures and markets high performance lasers for the scientific (laboratories and universities), industrial (manufacturing, defense, LiDAR sensors), and medical (ophthalmology).

For Raman applications, LUMIBIRD offers a wide range of UV, visible and infrared fiber lasers (from 0.35 to 2 µm). We offer single-frequency CW lasers and pulsed solutions with spectral linewidths of the order of a few pm. Our products have very good spectral properties thanks to a high OSNR (Optical Signal to Noise Ratio). Most of our products are available with polarisation-maintaining or random fibers and have very good beam quality ($M^2 < 1.2$).

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Since 2005, **CytoViva** has helped hundreds of research and industry laboratories solve critical problems at the nanoscale with its state of the art hyperspectral microscope technology. Research applications supported by CytoViva range from nanotechnology to digital pathology.

CytoViva provides hyperspectral imaging solutions from the visible to near infrared range, which are specifically designed to work with all modalities of optical microscopy. This includes CytoViva's patented enhanced darkfield microscope optics, fluorescence and standard brightfield microscopy.

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**Chromacity** is a world leader in the design, development, and manufacturing of advanced ultrafast pulsed fibre lasers. Based in Edinburgh, UK, the company specialises in fixed wavelength femtosecond fibre lasers and picosecond optical parametric oscillator (OPO) based tuneable laser systems. Based on a novel patented laser architecture that delivers ultra stable long-term performance, the fixed wavelength femtosecond fibre lasers work at 1040nm, 920nm and 520nm, and the tuneable picosecond OPO lasers operate across the near infra-red and mid infra-red wavelengths from 1.4um to 12um.

The lasers are used for scientific and industrial research including spectroscopy (materials analysis), microscopy (biological imaging), defect detection, pollution monitoring and a broad variety of quantum applications.

All Chromacity's lasers are compact, air-cooled devices, and offer unrivalled long term pulse stability without the need for on-going maintenance. The company sells its products either directly, or via a global network of distributors and agents.

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**S.T. Japan** stands as a premier global provider of spectra databases and cutting-edge sample preparation tools for microanalysis.

Operating on a global scale, S.T. Japan specializes in the creation and distribution of comprehensive spectra databases, covering ATR-FTIR, FTIR, Raman, and NIR, alongside advanced accessories tailored for analytical laboratory sample preparation. Our extensive database collection encompasses spectra for a wide range of materials, including polymers, solvents, pharmaceuticals, illicit substances, food additives, packaging materials, explosives, hazardous materials, forensics, minerals, petrochemicals, and more. These databases are thoughtfully developed to enable rapid and precise sample identification and are compatible with standard database formats.

Our state-of-the-art sample preparation tools, engineered and manufactured in Japan, are designed to meet the exacting requirements of efficient and dependable sample preparation in analytical laboratories. These tools are invaluable for users tackling the everyday challenges of sample preparation.

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# EXHIBITORS

**HORIBA Scientific** (www.horiba.com) provides an extensive array of instruments and solutions for applications across a broad range of scientific R&D and QC applications.

Our proven quality and trusted performance can be found in over 500 types of scientific analyzers for Raman spectroscopy, fluorescence spectroscopy, atomic force microscopy, X-ray fluorescence spectroscopy, elemental analysis, GDOES, ICP-OES, particle characterization, forensics, spectroscopic ellipsometry, sulfur-in-oil, surface plasmon resonance imaging (SPRi), water quality measurements, custom spectroscopy solutions and OEM spectroscopy components.

Our instruments are found in universities, industries, research institutions, and government agencies. HORIBA provides multi-faceted data solutions in some of the most advanced science and technologies – assisting the most cutting-edge research in uncharted territories, and fueling applications in life sciences, pharmaceutical, materials research, food and agriculture, environmental, energy, water etc.

In 2019 HORIBA has celebrated the 200th anniversary of its optical spectroscopy roots. The Maison Soleil was founded in 1819 by Jean-Baptiste Soleil, becoming in 1923 the company Jobin Yvon through association with Amédée Jobin and Gustave Yvon. The technical foundation given by the Maison Soleil and the subsequent Jobin Yvon company remains at the heart of HORIBA's spectroscopy products, which are renowned for their performance and quality.

**Cambridge Raman Imaging Limited** was founded in March 2018 with the idea to introduce fiber lasers to the biomedical market. With a combination of private and public funding, the company conducted extensive research and development to create a fast and high-resolution imaging solution that surpasses traditional biomedical imaging methods. In 2020, (we established a 100% owned subsidiary, CRI S.r.l, in Italy to expand our global outreach and accelerate the commercialization of our technology.

Today, Cambridge Raman Imaging Limited is a key player in the field of biomedical imaging, with a growing network of customers and partners across the world, and we are committed to continue pushing the boundaries of biomedical imaging.

www.cambridgeramanimaging.com

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**Opton Laser International** (www.optonlaser.com) was established in 1990 and has become a key supplier to the photonics market, offering a rich selection of innovative products within a totally independent, flexible and responsive organization. Opton is a fast growing company located in Les Ulis, France, and has gained an international reputation for competence and stability. Long term partnerships with market leaders have strengthened Opton position in the French market, particularly in the fields of lasers, spectroscopy, laser instrumentation, signal processing and micro-positioning. Opton recently extended its activity to French speaking Switzerland. Opton supplies a variety of systems for vibrational spectroscopy, including innovative high speed MIR spectrometers and fluorescence free Deep UV Raman systems and is very proud to have been selected as the exclusive French distributor of Lightnovo to address the Raman spectroscopy market with more innovative solutions.

Lightnovo has developed a full range of Raman spectrometers and microscopes that can be summarized in three product lines: miniRaman, RG and Thor.

- miniRaman is an advanced miniaturised Raman spectrometer with an integrated, patented, reference channel. This technology allows for automatic calibration of the unstabilised laser wavelength drift. The spectrum from the sample gets always corrected for Raman shift and Raman intensity. This allows for a continuous calibration of the device and, therefore, the results are fast and reliable. This feature makes miniRaman the most compact Raman spectrometer on the market while ensuring very high performance, making it an ideal and affordable solution for materials identification and quantitative measurements. miniRaman spectrometer can be used as a module for a fully automated microscopy platform for advanced Raman mapping at the world smallest footprint.

- RG Raman spectrometers and microscopes provide enhanced spectral resolution (down to 1.5 cm-1) and extended spectral range (down to 50 cm-1) for demanding applications in material, chemical and biological sciences.

- Thor microscope has patented artefact-free polarized Raman microscopy features that allow quantitative orientation mapping similar to electron microscopy.

To find the best product for your application or for a trial of the instrument, please contact jean-paul.gaston@optonlaser.com if you are in France or sales@lightnovo.com outside France.

# SPEAKERS INDEX

## Deep Jariwala

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# Nanomaterials Characterization for Functional Devices: The role of Raman Spectroscopy

Abstract (Arial Narrow 12)

Low-dimensional nanomaterials have made their way into several technologies and applications. However, new materials and new applications of the same continue to emerge. In this talk, I will focus on several such examples comprising 2D semiconductors[1-4] and 1D semiconductors[5]. I will specifically highlight how near-field and far-field optical spectroscopy and Raman Spectroscopy can be valuable tools in characterizing such materials for fundamental understanding of their opto-electronic properties and also their applications into functional devices.

I will end the talk with a broad perspective on the need to rapidly and accurately characterize nanomaterials and their interfaces and why that is critical for future applications in the semiconductor industry.

## References

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[2] *ACS Nano* **2024,** 18, 17958–17968
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[4] *Nano Letters* **2024**, 24, 4725–4732
[5] *Nature Photonics*, **2024** DOI: 10.1038/s41566-024-01504-0

# Giulio Cerullo[1,2]

## Dario Polli[1], Matteo Negro[2]

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# Broadband stimulated Raman scattering microscopy

Stimulated Raman scattering (SRS) microscopy is a powerful nonlinear optical technique for chemical identification of (bio)-molecules based on their intrinsic vibrational spectrum, which allows high-speed label-free imaging of cells and tissues. It is based on the combination of two narrowband laser pulses, the pump and the Stokes, whose frequency difference matches a vibrational frequency, and the measurement of the Stokes beam amplification (stimulated Raman gain, SRG). Single-frequency SRS microscopy allows the detection of molecules with a specific Raman response but is not sufficient to distinguish different components within complex heterogeneous systems in which chemical species display spectrally overlapped resonances. For this reason, there is ongoing research aimed at extending SRS to broadband detection, combining the speed of coherent Raman spectroscopy with the information content of spontaneous Raman [1]. Broadband SRS is however technically challenging, as it requires simultaneous detection of the tiny SRG signal at multiple wavelengths simultaneously. In this talk we present a broadband SRS system specifically designed for deployment in a biomedical environment, for both research and clinical applications. The system starts with an intrinsically synchronized all-fiber laser, generating a narrowband pump and a broadband Stokes, with frequency detuning covering the CH stretching region (2800-3100 $cm^{-1}$). A home-built high-frequency multichannel lock-in amplifier is then used to simultaneously measure the SRS signal over 38 frequencies simultaneously [2], covering the CH stretching band with 10-20 µs pixel dwell time and allowing for detailed, high spatial resolution mapping of spectrally congested samples [5]. We demonstrate the performance of our SRS microscope by high-speed, label-free, non-destructive imaging of senescent cancer cells and liver tissues of mice subject to non-alcoholic steatohepathitis (NASH, Figure 1).

## References

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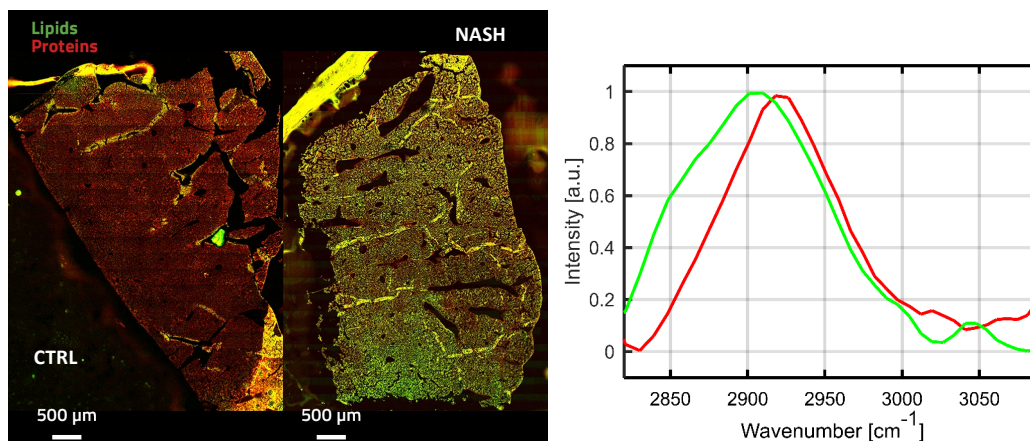


**Figure 1:** Left panel: SRS images of tissue samples from the liver of a mouse affected by the NASH disease (right) as compared to a control sample (left). Pixel dwell time: 20 µs. Right panel: SRS spectra of lipids (green) and proteins (red).

## Pr. Ludovic Duponchel

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# LIBS and Raman image fusion: An original approach based on the use of chemometric methodologies

Laser-induced breakdown spectroscopy (LIBS) imaging is an increasingly popular and powerful technique across many scientific fields. LIBS imaging allows for the detection of atomic elements in complex samples, providing crucial spectral and spatial information. Key advantages of this method include minimal sample preparation, high acquisition speeds of up to 1 kHz, high spatial resolution (on the micron scale), and sensitivity in the ppm range. Another significant benefit of current LIBS systems is the ability to perform additional spectroscopic analyses, such as Raman measurements, on the same platform.

Traditionally, LIBS imaging data has been analyzed using univariate approaches, focusing on maps at specific LIBS wavelengths. However, this method limits the extraction of the full range of information available in the spectra, hindering a comprehensive understanding of the relationship between spatial and spectral data. Chemometrics and multivariate analysis, particularly spectral unmixing, can address this limitation.

This presentation aims to demonstrate the potential of simultaneously analyzing LIBS and Raman imaging data from the same sample using the Multivariate Curve Resolution – Alternating Least Squares (MCR-ALS) unmixing method [1]. To showcase the value of this integrated analysis, we apply it to a complex polymetallic mineral containing carbonates, silicates, and sulfides. We will show that by using a data analysis pipeline previously validated by our group, we can extract the pure chemical contributions of these heterogeneous minerals. While the presented protocol is effective for analyzing LIBS and Raman data separately, it is far more insightful when both datasets from the same sample are analyzed together, revealing new insights that would be missed without this integrated approach.

## References

[1] A. Nardecchia, A. de Juan, V. Motto-Ros, C. Fabre and L. Duponchel, Spectrochimica Acta B, 198 (2022).

Senada Koljenović[1,2]

Yassine Aaboubout[2], Omid Elahi[1], Sebastiaan Van Der Auwera[1], Karen Zwaenepoel[1], Koen De Winne[1], Louis Delsupehe[1], Klaas De Corte[1], Hetty Mast[2], Ivo ten Hove[2], Aniel Sewnaik[2], Jose Hardillo[2], Dominik Monseres[2], Gilles van Haesendonck[1], Steven Mariën[1], Willem Lybaert[1], Callum Faris[1], Wouter De Vos[1], Martin van der Wolf[3], Tom Bakker Schut[3], Rosa Soares[3], Gerwin Puppels[3]

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# Improving oral cancer surgery by intra-operative assessment of resection margins: need for objective techniques

Patients with oral cavity cancer are often treated with surgery. **Of the many factors that may affect the clinical outcome of patients with OCSCC** (such as tumor site, TNM classification, patient age, comorbidity) **only the resection margin is under the control of the surgeon and the pathologist.** The goal is to remove the tumor with a margin of > 5 mm of surrounding healthy tissue, according to the international guideline of Royal College of Pathologists. This results in the best patient outcome through highest 5-year survival, less need for adjuvant radiotherapy/chemotherapy, better quality of life, less tumour recurrence. This is referred to as "adequate surgery". However, in the oral cavity region many important and delicate functional tissue structures should be spared if possible. Moreover, it is often impossible for the surgeon to accurately delineate the tumour in the operating room by visual inspection and palpation alone. Unfortunately, as a result only about 15% to 26% of the oral cancer surgeries achieve adequate resection margins. **Intraoperative assessment of tumor resection margins can dramatically improve surgical results**. It enables the surgico-pathological team to directly perform additional tissue resection, if necessary, to achieve a so-called **"first time right surgery"**. However, current methods are laborious, subjective, and logistically demanding. This hinders broad adoption of intraoperative assessment of tumor resection margins, to the detriment of patients. Inadequate resection margins result in the need for a 2nd, sometimes 3rd operation, combined or not with chemotherapy or radiotherapy. **Therefore, an objective easy-to-use technique is needed**, to accurately assess all resection margins intraoperatively. The challenges in pathology and the opportunities of photonic techniques in general will be discussed. The development of a high-wavenumber Raman spectroscopic technology, for quick and objective intraoperative measurement of resection margins will be presented.
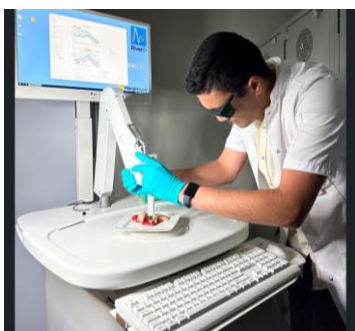


**Figure 1:** Raman spectroscopy-based intra-operative assessment of resection margins during oral cancer surgery

# Sara Abalde-Cela

Dr. Sara Abalde-Cela, International Iberian Nanotechnology Laboratory (INL), Avda Mestre José Veiga s/n, 4715-310, Braga Sara.abalde@inl.int

## SERS-based optofluidic platforms and spectromics for health applications

In the past 20 years, the microfluidics community developed extremely advanced systems able to perform almost any chemical and/or biological lab protocol. However, to develop integrated lab-on-a-chip diagnostic platforms, it is crucial to couple microfluidic devices with detection strategies able to match the inherent properties of microfluidics: high-throughput, automation and miniaturisation.[1] One of those detection techniques is surface-enhanced Raman scattering (SERS) spectroscopy, an ultrasensitive and highly selective analytical technique with multiplexing ability. Despite all its advantages, the struggle of SERS in translational medicine and its transfer into clinics may be based on many factors, including, but not limited to, the cost and reproducibility of SERS substrates and the lack of standardization and benchmarking of SERS platforms. The integration of SERS with microfluidics allows miniaturisation and automation, reducing acquisition times and inter-test variability for complex biological samples analyses. [2] We have shown how the integration of different SERS sensing substrates and strategies within microfluidics and microdroplets offers a great flexibility for the diagnosis of several biological species and/or events. In this talk, I will show examples demonstrating the potential of SERS-based optofluidic platforms for single cell multiplex phenotypic analysis, for the differentiation of cancer versus healthy cells or for the metabolomic analysis for metastasis prediction.[3] These approaches may be transferred to different analytical fields, such as the detection and discrimination of foodborne pathogens, bacteria or viruses in food or water samples.

### References

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[2] Kant, K. et al., (2024), Nanoscale Horizons, in press.
[3] Oliveira, K. et al, (2023), 11, 2201500.

### Figures
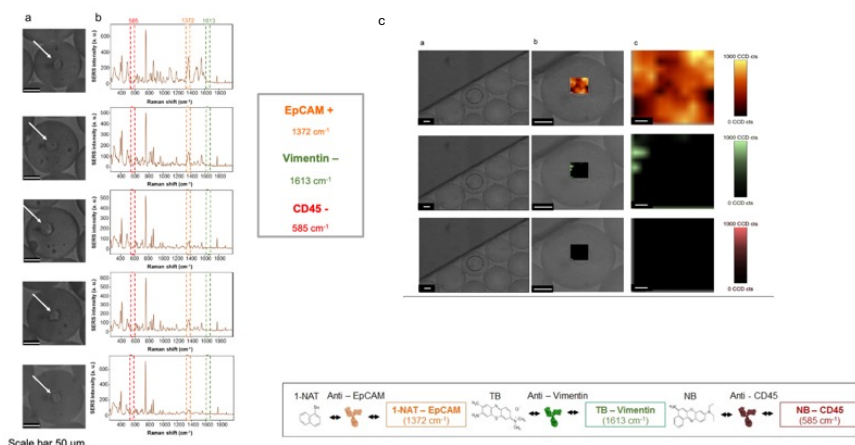


**Figure 1:** SERS-based phenotypic detection of isolated single cancer cells in microdroplets and multiplex analysis for the presence/absence of cell membrane proteins and corresponding cell surface intensity mapping for protein expression distribution.

# Miguel A. Bañares

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# *Operando* Raman methodology, getting a grip on structure-performance of working functional materials: the catalysis instance

Understanding functional materials at a molecular level is connecting its performance with the structure it has during operation. The concept behind *operando* methodology is that the functional material must be characterized while working in an array that allows simultaneously measuring its performance free of distortions imposed spectroscopic cell features. The working condition of some functional materials are of different nature; touching base in the case of catalysis, this requires reinventing the spectroscopic cell from a cell where you mimic reaction conditions. This is a generalized change of gears in catalysis science [1]. Since it was first proposed in literature in 2002, with three papers [2][3][4], there has been an exponential growth on its use with more than 1070 papers in 2023 (Scopus). An *in situ* study will report on the state of the catalyst while working but will fail to report what is the real catalytic performance. The operando methodology for catalysis requires taking spectroscopy to the catalytic reactor rather than bringing the catalytic reaction to an *in situ* cell. We will present how *operando* reactors are and show Raman *operando* instances that simultaneously report changes in the catalyst structure/surface species and on its performance.

Along with experimental rigs, *operando* Raman methodology need detailed spectral analyses and may in turn be used for process control. Hence, within CHARISMA project, we are working not only on harmonization of Raman spectra, but also on adapted data formats that include all process and processing metadata. These approaches are relevant for research made in other applications.

## References

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# István Csarnovics

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# Peculiarities of using different nanostructures for surface-enhanced Raman scattering

Raman spectroscopy is a branch of vibrational spectroscopy that allows highly sensitive structural identification of various chemical and biological materials based on their unique vibrational characteristics, all without destroying the sample. Raman spectroscopy is an effective tool for analytical studies, but the low intensity of Raman signals is a significant disadvantage of the method.

The surface-enhanced Raman scattering (SERS) method could enhance the light-matter interaction during the Raman process, mainly through nanostructures. The enhancement of the SERS process depends on the material, shape, and geometrical parameters of the nanoparticles while simultaneously on the excitation wavelength and the nature of the selected analyte. Different nanostructures (nanoislands, nanoparticles, nanotrees) were created and analyzed, and their parameters were optimized to obtain a higher enhancement factor and to determine the detection limit of the selected analyte. Also, the different creation methods were compared from the point of view of the sensing application. SERS is a commonly used technique to enhance the signal that allows the analysis of low-concentration samples or even the detection of a single molecule. The SERS effect can occur when the analyte is near a nanoscale-structured metal surface. By using metal surfaces with optimal parameters, the intensity of Raman signals can be enhanced by several orders of magnitude.

Our previous research shows that thermal dewetting of thin metallic layers could be used for SERS application. In this research, we compare the results obtained during the examination of nanostructures created by spark ablation and vapor-liquid-solid techniques to find the optimal creation parameters for the SERS substrate with a higher enhancement factor, which is suitable to detect the least analyte and will be ideal for further applications. Figure 1 shows the Scanning electron microscope images of different nanostructures for the SERS application.
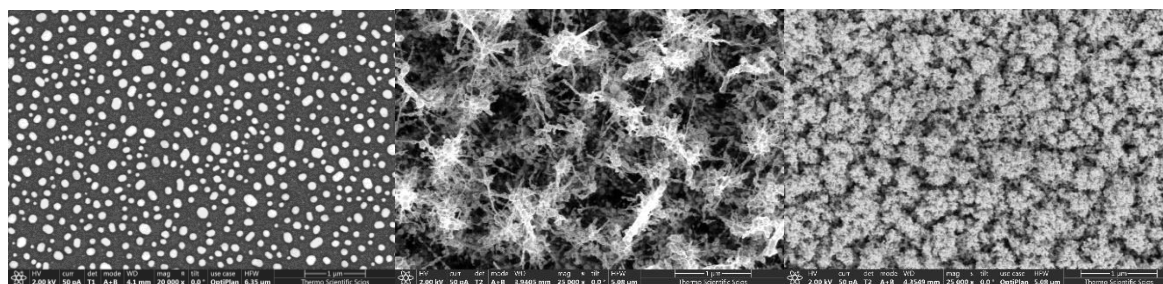


Figure 1: Scanning electron Microscope images of the created and investigated nanostructures: a) Thermal dewetted gold nanostructures, b) Carbon nanotrees covered by gold layer, c) Ag-Au gold nanostructures created by arc-discharge method.

# Yann Gallais

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# Ultrafast dynamics of quantum materials by time resolved Raman scattering

Controlling materials properties with light pulses is an emerging field in condensed matter research. Quantum materials with their delicate interplay of magnetic, electronic, orbital and lattice degrees of freedom offer an attractive playground to demonstrate optically induced novel phases out-of-equilibrium with unique properties.

To achieve this, spectroscopic techniques capable of probing electronic, magnetic and lattice degrees of freedom on the ultrafast timescales (picosecond or femtosecond), both table-top and in large scale facilities, are currently being developed. In this talk, I will discuss the extension of Raman scattering to the ultrafast time scale as a symmetry resolved probe of non-equilibrium lattice and electronic properties of quantum materials. Quite remarkably this well-established technique to probe quantum materials in equilibrium has remained relatively underused on the ultrafast time scale. After a brief introduction to the technique, I will illustrate its use to the candidate excitonic insulator material $Ta_2NiSe_5$. I will show that a metastable phase with unique lattice and electronic properties can be induced in this material by a sub-picosecond near infrared pulse. If time allows, I will also discuss more recent results on the out-of-equilibrium dynamics of superconducting cuprates.

## References

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## Figures
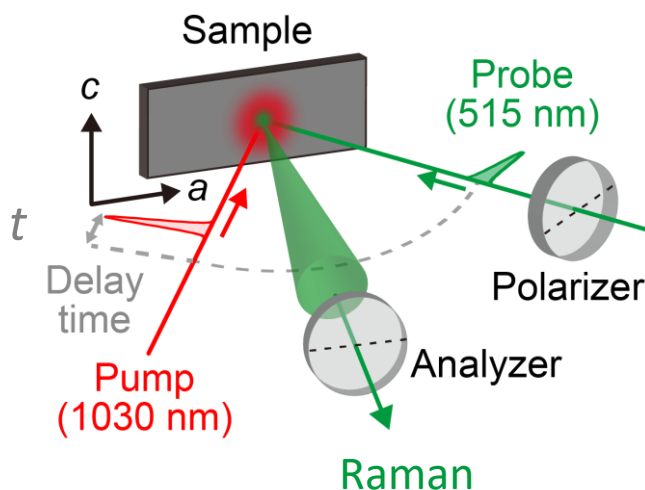


**Figure 1:** Ultrafast two-colour pump-probe Raman scattering

# Professor Pola Goldberg Oppenheimer

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## Advanced Handheld Spectroscopic Portable Technologies for Point-of-Care Neurodiagnostics

Traumatic Brain Injury (TBI) is a major cause of morbidity and mortality, with increasing incidence worldwide, causing long-term disability. After head trauma, critical decisions affecting patients' treatment and outcomes must be made rapidly. However, TBI is hard to diagnose at the point-of-care with many patients often exhibiting no specific clinical symptoms and remaining undiagnosed. The current lack of point-of-care diagnostics often results in incorrect patient management and causes avoidable cognitive, emotional, or physical morbidity. There is a clear urgent need for rapid portable point-of-care diagnostics technologies to enable timely intervention. We have developed a technology for rapid data acquisition of molecular Raman fingerprints of TBI biochemistry to safely measure proxies for cerebral injury through the eye, providing a tangible path towards non-invasive point-of-care neurological diagnostics using simultaneous Raman spectroscopy and fundus imaging, packaged as a low-cost, hand-held device, analysing the neuroretina and optic nerve, as a projection of the central nervous system. This device exploits the optical properties of the eye to focus a harmless collimated sensory beam onto the optic nerve and retina to instantaneously detect TBI-related biochemical changes. To demonstrate the capability to detect endogenous neuromarkers in murine and porcine neuro-retina, our portable and eye-safe device was optimised and tested on an eye phantom, which mimics the optical and spectral characteristics of the eye. Subsequently, testing on the porcine eye posterior detected an enhancement of high-wavenumber bands via the 633nm excitation laser, whilst in the murine eyes, the most intense peaks detected suffered little interference exhibiting a clear separation between TBI and healthy cohorts, further classified using our advanced artificial neural network (ANN) algorithm, which enabled an automated interpretation of Raman data. Clinically, this ANN decision support translates into reduced reliance on specialist support, dramatically improving the speed and cost of diagnosis. Designed as a handheld cost-effective platform, the developed technology can allow clinicians to rapidly assess TBI at the point-of-care including, at the roadside, or pitch-side and can also be used to quantify long-term brain injury, identify changes in brain biochemistry or function due to acute or chronic neurological diseases.
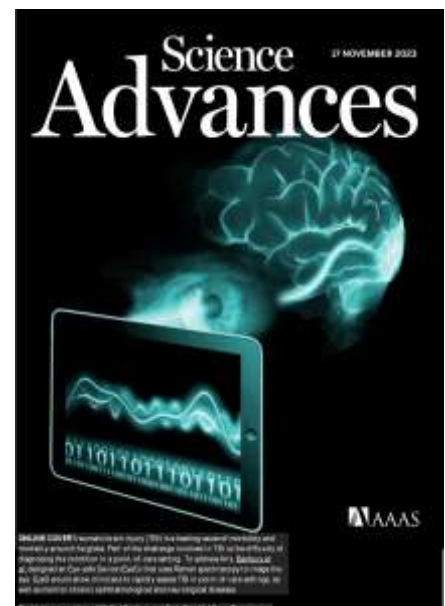
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# Raman Reporters Derived From Aryl Diazonium Salts for SERS Encoded-Nanoparticles

Sensing and imaging technologies based on the use of nanoscale tools have received growing interest these last decades. Among the portfolio of reported bioimaging nanotools, labels based on optically encoded metallic nanoparticles (NPs) are particularly attractive as they are efficient Raman signal enhancers, giving rise to intense surface-enhanced Raman spectroscopy (SERS) signatures. The rising popularity of SERS tags in recent years has made them a compelling alternative to fluorescent probes, thanks to their distinctive advantages. Indeed, unlike the broad spectral profiles associated with fluorescent probes, SERS tags produce multiple sets of narrow peaks, resulting in minimal spectral overlap and exceptional multiplexing capability. In this talk, we will describe the potential of aryl diazonium salt-encoded gold or silver nanoparticles as contrast agents for Raman imaging[1-3]. Compared to the commonly used thiol self-assembled monolayers for SERS tag preparation, aryl diazonium salts offer several key advantages: (i) they form robust interfacial bonds with the supporting NPs, (ii) they generate intense SERS fingerprints, and (iii) they allow for the creation of multifunctional layers. These multilayers have been utilized to incorporate multiple SERS labels along the grafted polyaryl chains and introduce post-functionalization sites. Thanks to this strategy, anticounterfeiting inks could be prepared and deposited using additive printing techniques, such as inkjet printing. This next-generation of SERS-encoded NPs has been investigated for its potential applications as optical nanosensors, anticounterfeiting agents, and contrast agents for SERS bioimaging (see Figure 1).

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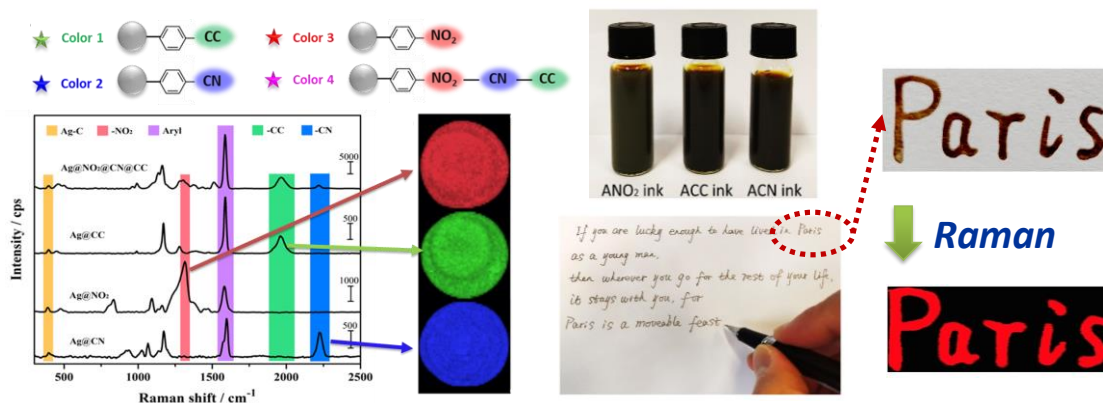


**Figure 1:** Illustration of SERS-encoded NPs functionalized by diazonium salts along with their SERS spectra and images (left-hand side). Picture of the anti-counterfeting inks and corresponding optical and Raman images (right-hand side).

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# Standardization and Harmonization Effort on Microplastics Analysis by Spectroscopic Methods.

Plastic pollution is recognised as a severe anthropogenic issue globally, where complex physio-chemical transformation processes (such as aging, degradation and fragmentation) producing Microplastics (MPs, 1000-1 µm) and, subsequently, Nanoplastics (NPs, <1 µm). Plastic debris comes in a huge range of sizes, polymer types, levels of physicochemical degradation and associated chemicals, therefore a combination of different sampling, sample processing and analytical techniques is needed. To date, many different analytical protocols, methods and techniques have been developed and applied to samples containing multiple polymer types and certain fractions of particle size. However, validated standardized methods remain unavailable at this point.

The most common techniques to reliably identify MPs are micro-Spectroscopy (Infrared or Raman) or Thermo-Analytical methods [1]. While the mass-based thermo-analytical methods can determine the overall mass of different polymer types (LOD in the µg range), the particle-based spectroscopic methods provide information on the polymer type, number, size and size distribution, and potentially identify a single polymer particle in the sub-micron range. While several studies provided a path forward to harmonization, there is an urgent need for collaborative method development, (certified) reference materials and inter-laboratory studies (ILS) to validate and harmonize the various methods (including how to report results) [2]. These efforts and tools are needed to enable a better assessment of data quality and to develop a more efficient and reliable measurement infrastructure in support of (i) ECHA's proposed restriction targeting intentionally added MPs in consumer products, (ii) the Marine Strategy Framework Directive (MSFD), (iii) the new Drinking Water Directive (DWD) that mentions MPs explicitly, and (iv) the new Circular Economy Action Plan (CEAP) adopted in March 2020.

In this talk, an overview of the more recent standardization and harmonization activities will be presented, including i) European projects (eg. EUROqCHARM, 21GRD07 PlasticTrace) that critically review the state-of the-art of the analytical methods and take harmonisation one step further with the preparation of suitable reference materials for QA/QC and harmonisation of methodologies; ii) ILC studies to validate the performance of spectroscopy methods (µ-IR, µRaman) and thermogravimetric methods (eg. VAMAS TWA45); iii) International initiatives and cooperation at the ISO level (eg. ISO/TC 147/SC 2/JWG 1) to set out the key principles for the investigation of microplastics in drinking water and water with low content of natural suspended solids using vibrational spectroscopy, with a main focus on sample preparation, measurement methods, data processing, and method validation.

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# Skin barrier function characterization by Raman spectroscopy: from in vitro to in vivo

Skin is a complex, multilayered organ which covers and protects the surface of human body against water loss and exogenous agents. Remarkable efforts have been developed in cutaneous research for: i/ the understanding of skin homeostasis, ii/ the characterization of a physiological and a physio-pathological status, and iii/ the detection and the evaluation of the impact of endogenous or exogenous particles within the skin.

Raman spectroscopy is becoming increasingly popular providing information on the organization, the conformational order for lipids, secondary and ternary structure for proteins the state of water mobility in the skin…. Raman has the advantage to provide a similar level of information in vitro, ex vivo and in vivo.

The talk displays a combined or parallel use of vibrational and separative techniques coupled to mass spectrometry for the characterization of the skin barrier in physiological or physiopathological states. Short examples highlight obtaining molecular understanding at in vitro, ex vivo and in vivo levels; as well as the use of Raman to follow-up drug permeation and the correlation with the evolution of the lipid's composition and their organizational order.

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# Structural battery electrolytes: effect of composition on physico-chemical properties

Structural batteries have emerged as promising multifunctional composites in the field of Li-ion batteries. They consist of interpenetrated, multifunctional components: (*i*) carbon-fibers that enable the intercalation of lithium ions and provide electrical conductivity and mechanical reinforcement, and (*ii*) a polymer network that transfers mechanical load while confining (*iii*) the liquid electrolyte responsible for ion transport.[1] With their unique design, structural batteries represent the next generation of load-bearing components for electric transportation, offering lightweight storage of electrical energy throughout the structure of a vehicle. Developing these batteries is crucial for reducing emissions by improving fuel efficiency. For an optimal performance, suitable structural battery electrolytes need to be designed to enable sufficient mechanical load transfer and long-range ionic transport between the electrodes.[1]

In this study, Raman spectroscopy was employed to gain deeper insights into the intermolecular interactions among the various components of the system. The collected Raman spectra were analyzed across three distinct regions: the lower spectral range (240-450 cm$^{-1}$), sensitive to TFSI conformational changes; the middle spectral range containing a strong vibrational mode at $\simeq 743$ cm$^{-1}$, attributed to the expansion-contraction mode of the entire TFSI anion ($v_s$ S-N-S and $v_s$ CF$_3$), which correlates with the TFSI anion coordination; and the spectral range (1550-1650 cm$^{-1}$), where the degree of curing of the methacrylate-based polymer was estimated. The collected Raman data were then correlated with morphological, thermal and relaxation dynamics data to highlight the fine tunability of the structural battery electrolyte properties with composition.

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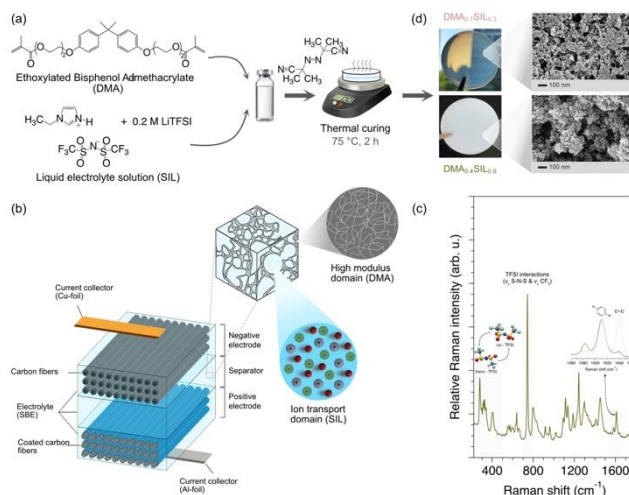


**Figure 1:** (a) Details of the SBEs synthesis procedure; (b) Illustration of the SBEs concept; (c) Raman spectra of the SBEs collected at RT; and (d) SEM images of the cross-section of samples DMA$_{0.7}$SIL$_{0.3}$ (top) and DMA$_{0.4}$SIL$_{0.6}$ (bottom).

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# The use of Raman spectroscopy for quality analysis of hydrogen

The optimal functioning of fuel cell vehicles requires the use of high-purity hydrogen (ISO 14687), as impurities can cause both temporary performance issues and irreversible damage. However, production processes, such as vapor reforming, are not the only source of impurities. Contaminants can also be introduced into the hydrogen during subsequent steps its lifecycle. Therefore, it is important to conduct final quality checks at the nozzle to ensure that vehicles are refueled uncontaminated hydrogen. Traditional analytical techniques for assessing hydrogen quality require laboratory-based procedures, making them unsuitable for on-site implementation. In response to this challenge we present a newly developed Raman spectrometer for detecting these impurities. The utilization of small components results in a transportable and robust spectrometer, which allows the analysis of on-site analysis of hydrogen. This development allows a simplified calibration process and operation. The spectrometer is capable of detecting all relevant molecules listed in the ISO 14687 standard, which is shown in this study. This advancement has the potential to streamline the quality control process and facilitate rapid quality control with minimal delay. The presence of a gas matrix can be identified with minimal effort, typically within a few seconds.

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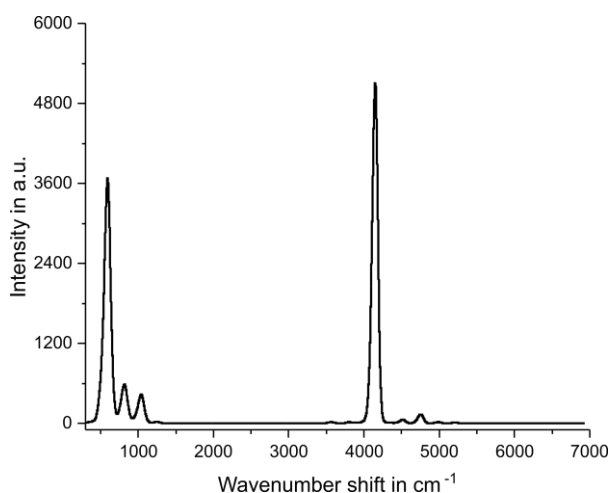


**Figure 1:** Exemplary spectrum of gaseous hydrogen, excited with a low cost 450 nm laser source. The vibrational as well as the rotational Raman bands are apparent.

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# Innovative Optical sensor based on gold nanostructures for Detection of Thiol-Containing Molecules in Blood

This project aims to revolutionize blood tests by introducing a novel method for precisely detecting thiol-containing molecules in blood samples. The proposed technique involves traditional Raman spectroscopy with the combination of SERS (Surface-enhanced Raman spectroscopy) overcoming the barriers of low concentrations, our technique relies on the incorporation of gold nanostructures into blood samples, triggering a unique reaction with thiol groups [1]. We hypothesize that this reaction emits detectable light within a specific Raman shift [2]. Our focus lies on selecting a medically significant thiol-containing molecule for detection, with preliminary emphasis on Cathepsins due to their high cysteine concentration, potentially providing increased specificity for accurate results. Targeted molecules include hormones implicated in diseases such as diabetes [3], obesity, autism, and cancer[4]. The project's interdisciplinary nature combines biomedical knowledge with engineering principles to address the need for faster and more efficient blood tests. This research has the potential to impact diagnostic procedures significantly, advancing the field of biomedical engineering while addressing critical challenges in blood testing.

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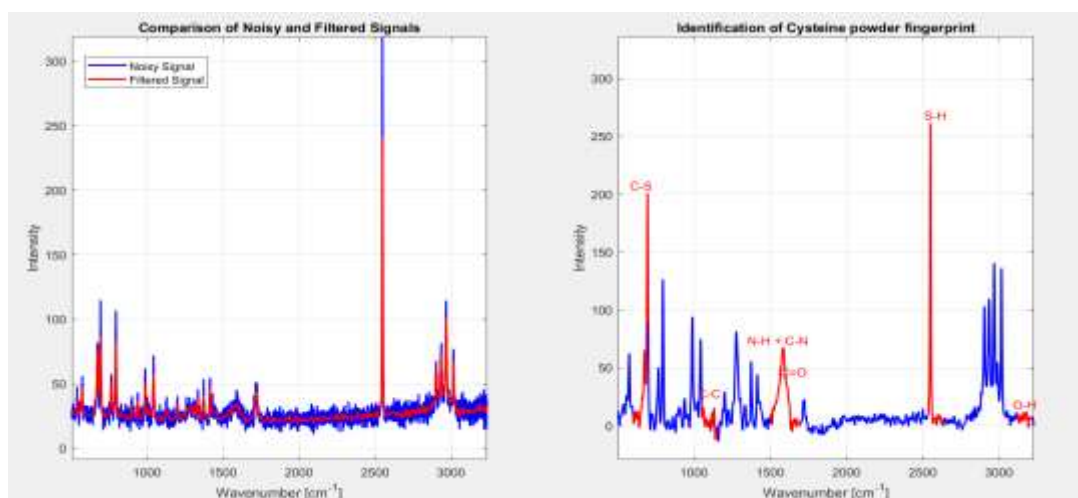


**Figure 1:** Original signal (in blue), filtered signal (in red), peaks related to certain structural bonds

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## Bubble-Assisted Laser Tweezers Raman Spectroscopy

Abstract: Raman Spectroscopy has been used for selective and sensitive detection of biomolecules for the last decade [1]. The development of Laser tweezers enables the nanoparticles to push against the wall of a microfluidic chamber to form strong SERS active clusters of nanoparticles. Obtaining Raman signals by trapping nanoparticles and controlling their activity through spatial assignment is known as Laser Tweezers Raman Spectroscopy (LTRS) [2]. A periodic array of such clusters can be designed by generating bubbles precisely focusing the laser on the glass substrate, known as bubble pen lithography (BPL) [3]. But, strong photoluminescence from the glass surface becomes much more prominent which debarred to obtain the Raman signal from a probe. This can be minimized by enhancing the plasmonic interaction between the gold nanoparticle and the substrate containing graphene oxide (GO) giving rise to a more intense SERS signal. In this context, we develop a new SERS substrate by electrospinning a polymer GO composite on glass/ quartz. We use this polymer surface to grow gold clusters with BPL. Now shining on the individual clusters with the Raman laser, we have an exceptional increase in the SERS signal, leading to greater sensitivity. In essence, the work demonstrates an elegant combination of BPL with LTRS to develop a sensitive technique to detect biomolecules in a very subtle amount.

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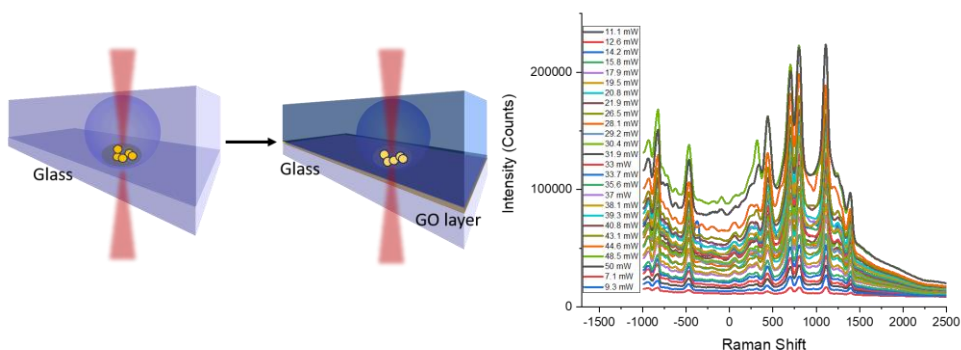


**Figure 1:** Bubble-assisted LTRS: A method to obtain systematic SERS response

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# Evaluation of an articular cartilage degradation level with use of Raman spectroscopy

Osteoarthritis, a leading cause of disability worldwide, causes permanent alterations in joint tissue structure. The diagnosis with existing methods usually occurs at an advanced stage, where tissue damage is extensive, leaving joint replacement as the only viable treatment. An early diagnosis could facilitate the initiation of drug therapies to decelerate joint degradation [1-3]. Our research group is focusing on creating an osteoarthritis diagnostic technique through Raman spectroscopy. Additionally, we're developing novel copolymers with a molecular bottlebrush structure for application at various levels of advancement of the degenerative disease. These proposed copolymers aim to act as lubricants in the affected joint, minimizing friction and warding off further damage.

This study aims to explore the link between the structure of articular cartilage and the progression of osteoarthritis. Through Raman spectroscopy analysis of cartilage tissue samples from several patients undergoing joint replacement surgery, we aim to investigate the association between various spectral parameters and the chemical compositional changes in cartilage as it degrades. Identifiable Raman bands of hydroxyapatite, chondroitin sulfate, and amide III groups were used to gauge the level of mineralization and remodeling in the cartilage tissue [4]. The insights gained will contribute to creating an index to measure osteoarthritis severity. Future work entails conducting in vivo experiments using a portable Raman spectrometer equipped with an endoscopic fiber optic probe. This device will allow for the direct evaluation of the joint interior during arthroscopic surgery.

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# Raman Spectroscopy of Gasses using Hollow Core Micro-Structured Optical Fibres

ISI have been working in collaboration with the Optoelectronics Research Centre (ORC) at the University of Southampton to develop a flexible on-line gas detection instrument with high specificity and sensitivity that can measure several gas species simultaneously, **Figure 1** - LHS. The Raman spectroscopy-based system uses a state-of-the-art hollow core fibre (HCF), a micro-structured silica fibre with a tubular hollow core which can be filled with the sample gas. The HCF facilitates an extended interaction pathlength between the excitation laser and the confined gas thereby enhancing gas measurement sensitivity. This approach also demands only very small sample volumes (microlitres).

Using the prototype design, a test program was funded through the SBRI on demonstrating the quantification of gas species of interest to the nuclear industry, ranging from simple diatomic gases e.g. $H_2$ to potential contaminants such as heteronuclear vapor phase organic species. Results showed excellent linear response across the target concentrations and the potential for low limits of detection. Another recent project targeted the detection of component species within a natural gas/ hydrogen blend sample. Ethane, methane, and hydrogen were all successfully detected using the HCF based Raman technique. The instrument development is currently focused on enhancing the limit of detection (LoD), by changing properties of the HCF and some mechanical variation in optical components, the current LoD is estimated at <2ppm, a 10ppm methane sample can been seen in **Figure 1** – RHS.

ISI is currently working on an SBRI UK funded project for the analysis of tritium in the nuclear fusion sector. In collaboration with Jacobs and the ORC, and funded through the Fusion Industry Program, ISI aim to demonstrate reliable performance in a variety of demanding deployment scenarios for this sector, as well as ensuring the compatibility of the instrument in the required environmental conditions.

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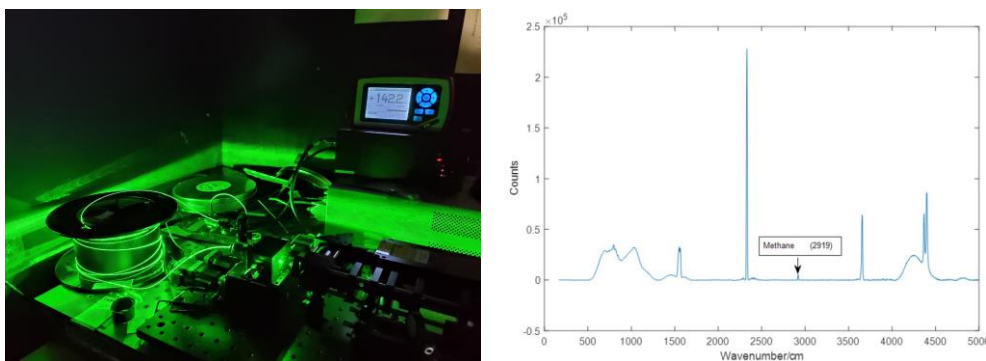


**Figure 1:** The gas Raman instrument (LHS) and the Limit of Detection testing, Raman spectrum showing 10ppm methane detection (RHS)

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# Raman Peak Analysis and Assignment in Conjugated Polymers

Conjugated polymers have vast applications across biosensors, drug delivery systems, organic electrochemical transistors (OECT), organic photovoltaics (OPV), organic emitting diodes (OLED), and thermoelectric generators (TEG).[1] These organic materials, are macromolecules characterized by an alternation of double and single bonds on their backbone, making them ideal candidates for various optoelectronic applications. By introducing electron-rich or electron-poor molecular units, one can effectively introduce electrons or holes into the polymer, thus fine-tuning its properties and enhancing performance.[1]

One of the advantages of these polymers is the fact that they are Raman active. This makes it possible to stut study of various components, including the backbone responsible for conjugation and any introduced side chain modifications aimed at tuning solubility or studying the doping gradient of electrically programmed channels.[2-3] Furthermore, Raman Spectroscopy extends to include the examination of transitions occurring within these materials. It is well-documented that organic compounds often exhibit multiple glass transitions, indicative of structural alterations across varying temperature regimes.

In this work, we attempt to analyze these transitions, distinguishing structural changes within the transition range performing Raman at variable temperatures. Such insights prove invaluable in understanding the dynamic behavior of these materials, giving us the opportunity to design strategies for enhanced performance optimization. Thus, Raman Spectroscopy emerges not only as a powerful analytical tool but also as a gateway to unlocking the full potential of organic materials across numerous applications, ranging from optoelectronics to biomedicine.

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## Cutting-Edge Solutions: Like a Pocket Knife, But for Your Lab

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# Raman Spectroscopy Investigations on Carbon Dioxide Sequestration through Wet Carbonation of Ca and Mg Silicate-Rich Minerals

The rise in carbon dioxide ($CO_2$) emissions from fossil fuel combustion has become a significant environmental concern, necessitating urgent global action to mitigate climate change. The Paris Agreement, established in 2015, aims to limit the global temperature increase to well below 2°C above pre-industrial levels, with efforts to restrict the increase to 1.5°C. This agreement underscores the importance of balancing anthropogenic emissions with the removal of greenhouse gases.

To address this challenge, the widespread deployment of negative emissions technologies (NETs) and carbon capture and storage (CCS) is crucial [1, 2]. $CO_2$ sequestration presents a promising strategy for capturing emissions, particularly in industries such as cement production. Utilizing carbonated materials as Supplementary Cementitious Materials (SCMs) offers a dual solution by capturing emitted $CO_2$ and recycling it within the cement industry. Wet carbonation emerges as a promising method for mineral carbonation due to its rapid reaction rates in an aqueous environment. However, further research is needed to understand the chemical carbonation reaction mechanisms and enhance reaction rates.

This study focuses on the carbonation of wollastonite, a calcium silicate-rich material, and olivine, a magnesium silicate-rich material, and their carbonation processes. Various factors influencing $CO_2$ uptake and the chemical carbonation reaction mechanisms are explored. Raman spectroscopy is employed to study these chemical reactions, using Raman mapping, providing new insights into phase changes during wollastonite and olivine carbonation. Complementary methods such as X-ray diffraction (XRD), X-ray fluorescence (XRF), automated mineralogy (SEM-EDX), Calcimeter, and thermogravimetric analysis (TGA) are also utilized.

The findings reveal the occurrence of passive layer formation during wollastonite carbonation via a double carbonation process. Additionally, the study highlights the beneficial impact of grinding on wollastonite $CO_2$ uptake, attributed to both size reduction and mechanochemical activation. Remarkably, over 80 % of the estimated calcium oxide in wollastonite, with potential for carbonation, has been successfully carbonated. These findings offer valuable insights into the potential of wollastonite carbonation for $CO_2$ sequestration and demonstrate the effectiveness of Raman spectroscopy in investigating the carbonation process.

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# Developing an AI algorithm for Raman spectrum analysis

Raman spectroscopy detects molecular vibrations via photon scattering, while Surface-enhanced Raman spectroscopy (SERS) enhances signals using nanostructured metals like gold or silver. Our study focuses on developing an algorithm to identify mi17RNA signatures in blood, a complex medium where overlapping peaks present significant challenges. The process includes comprehensive data preprocessing techniques such as moving average, convolution, moving median, moving max, normalization, baseline correction, and deconvolution for noise reduction and signal enhancement. Calibration is performed to ensure accuracy and consistency across different datasets. The algorithm's performance is validated on diverse datasets, with results displayed through clustered models to accurately distinguish molecular species and variations. This research advances automated Raman spectrum analysis for applications in materials science and biomedical diagnostics.

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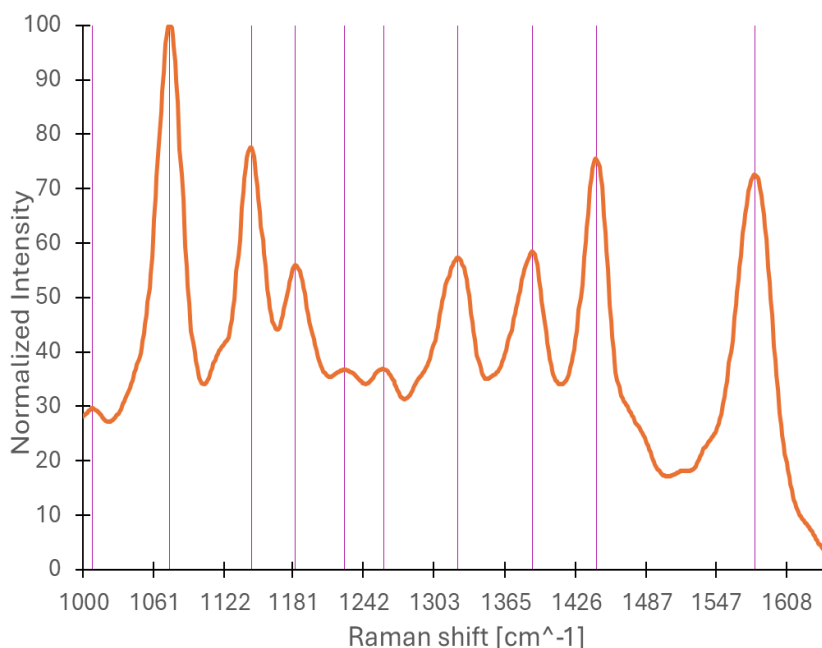


**Figure 1:** Normalized intensity (a.u) vs Raman shift ($cm^{-1}$), the Orange function represents the molecule 4-ATP after smoothing. the purple line represents the normalized model using a moving max window width of $n \pm 7$, with the parameter of the normalized threshold value set to 99.99 for peak detection resolution.

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# Transport properties of monolayer MoS$_2$ Functionalized with electro-active molecules

Two-dimensional (2D) materials have emerged as promising nanostructures for numerous applications ranging from electrocatalysis and optics to electronics and spintronics[1]. Among these, transition metal dichalcogenides (TMDs), such as 2D semiconductor MoS$_2$, have gained increased interest for their usage in electronics for high-performance field effect transistors (FETs) and diodes.[1,2]. Attaching molecular units to these 2D nanomaterials to finely adjust their physicochemical characteristics would add an additional degree of freedom. In this work, MoS$_2$ was functionalized by a ferrocene (Fc) derivative and thoroughly investigated by various characterization techniques, such as μ-Raman and XPS. Furthermore, conductive-AFM measurements were performed to investigate the effect of the chemical functionalization of MoS$_2$ on the electron transport properties.

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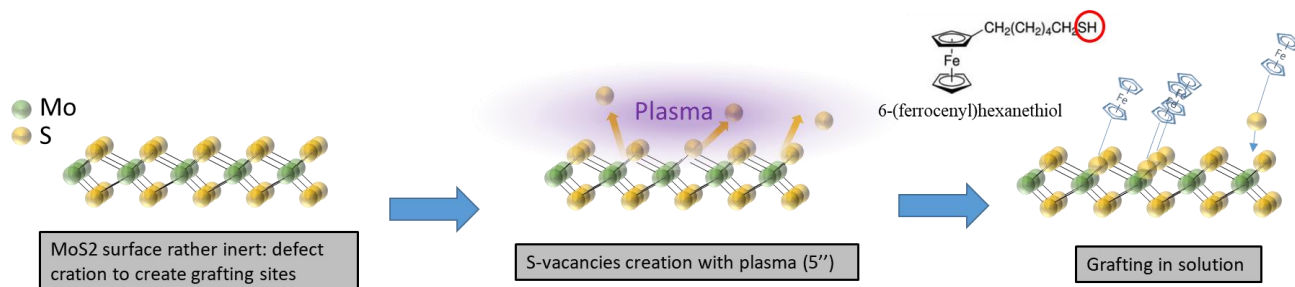


**Figure 1:** MoS$_2$ grafting steps

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# Optical nanofibers immersed in liquids for highly efficient Stimulated Raman Scattering

Optical tapered nanofibers (NFs) are fabricated by pulling fibers until reaching diameters comparable or smaller than the light wavelength (fig. 1, left). These devices are significantly exploited for a wide range of potential applications. Indeed, at such diameters, NFs exhibit a strong confinement of light in the silica which enables the generation of nonlinear effects. NFs can also present an intense evanescent field which has been exploited for optical sensing [1], optical traps [2] or spectroscopy [3]. However, the experimental investigation of optical nonlinearities in the evanescent field of the NFs remains limited. In this work, we present highly efficient and reproducible Raman converters built with a NF immersed in ethanol (fig. 1, right). The converters are pumped at 532 nm in the sub-nanosecond regime and the first Stokes order photons of ethanol are generated at 630 nm in the evanescent field probing the liquid. The Raman conversion operating range limited by the damage threshold is optimized, leading to an external Raman conversion efficiency up to 60% with a NF radius of 300 nm and a length of 8 cm [4]. Results obtained with other liquids such as toluene and propanol will also be presented. In addition to opening the way for a new family of all-fibered compact Raman sources, these devices can be exploited for applications in Raman spectroscopy of liquids or gases.

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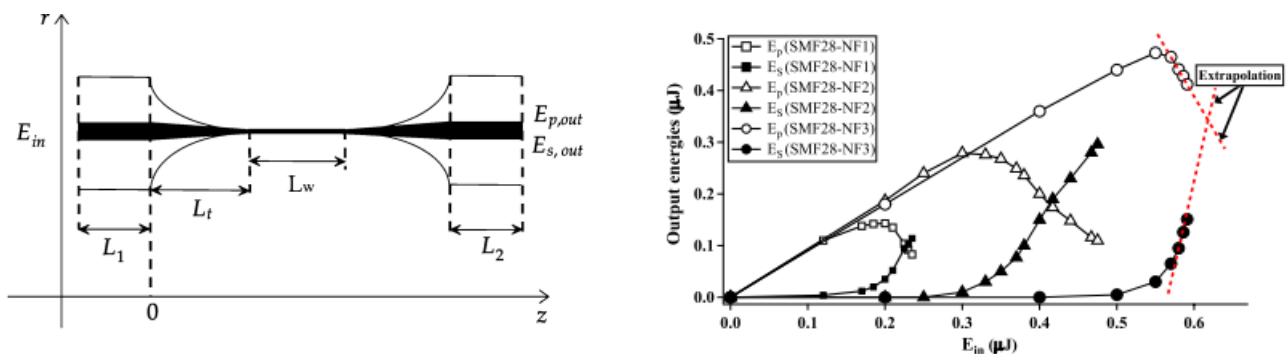


**Figure 1:** Left: Representation of a NF with its tapers. Right: Transmitted pump energy $E_p$ at 532 nm and output Stokes energy $E_s$ at 630 nm versus the laser incident energy $E_{in}$ for three different nanofiber radii $\rho$: SMF28-NF1 ($\rho$=220 nm), SMF28-NF2 ($\rho$=300 nm) and SMF28-NF3 ($\rho$=350 nm).

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# Cost-effective approach to fabricate highly sensitive surface enhanced Raman scattering (SERS) substrates

A low-cost, simple, repeatable method for obtaining Surface enhanced Raman scattering (SERS) platforms with an ordered distribution of gold nanoparticles and high enhancement Raman signal is presented. The platform is based on the decoration of Au / Ag nanoparticles into high-density Al nanoconcavities arrays. The nanostructured Al substrate follows a self-organized hexagonal pattern and are obtained by two-step electrochemical anodization of an Al substrate and the subsequent removal of the formed porous anodic [1-3]. The gold deposition time and the temperature and duration of the thermal annealing are determining parameters of the shape, size and arrangement of the gold nanoparticles formed on the Al templates alumina.

The size, shape, and arrangement of gold nanoparticles are dependent on the geometry of nanostructured Al substrates (nano-concavities, Figure 1) and the sputtering and thermal processes [4-6]. Also, a detailed evaluation of the different parameters of the fabrication steps is presented and how these platforms can be used as templates to create new SERS platforms with new features. The fabricated platforms have been demonstrated to be excellent sensing substrates for the detection of a broad range of molecules and medicines.

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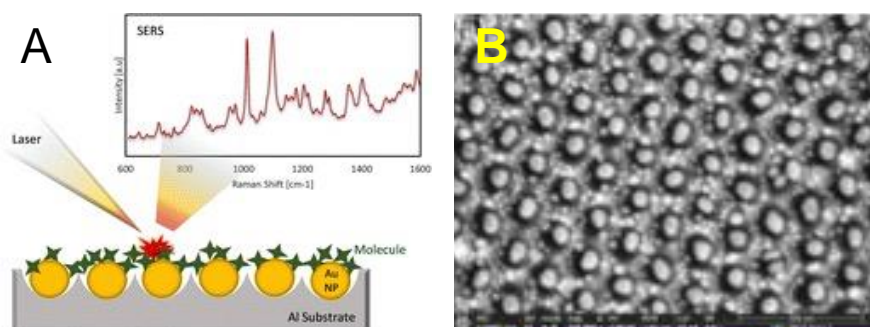


**Figure 1:** A) Scheme of Au nanoparticles arranged on Al self-ordered nanoconcavites as platform for SERS. B) FESEM image of the gold nanoparticles on Al nanoconcavities.

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# Dispersion studies of $VO_x$/$WO_x$/$TiO_2$ catalysts: the importance of combining Raman and IR spectroscopies

The emission of nitrogen oxides ($NO_x$) produced by fuel combustion poses a significant threat to both air quality and public health [1,2]. To address this problem, the current technology used to comply with the imposed restrictions is based on the selective catalytic reduction of $NO_x$, with $NH_3$ ($NH_3$-SCR) [3], where the $NO_x$ and $NH_3$ react in the presence of $O_2$, to produce $N_2$ and $H_2O$ [3–5]. The commonly used catalysts for $NH_3$-SCR in stationary plants and heavy-duty diesel vehicles are based on vanadium oxide supported on anatase $TiO_2$ with tungsten (W) used as promoter ($VO_x$/$WO_x$/$TiO_2$) [5].

This work utilizes Raman and infrared (IR) spectroscopy to study the dispersion of $VO_x$ and $WO_x$ species on the $TiO_2$ surface, a critical factor for catalyst performance.

Raman spectroscopy is commonly employed to evaluate the dispersion of $VO_x$ and $WO_x$ species on the $TiO_2$ surface and the corresponding monolayers through the identification of $V_2O_5$ and $WO_3$ crystalline phases, but distinguishing between V-O-V and V-O-W signals in mixed $VO_x$/$WO_x$/$TiO_2$ systems is challenging.

The use of resonance-enhanced Raman signals, alongside complementary IR data, provides valuable insights into surface species distribution.

Our results indicate crystalline phases of $V_2O_5$ and $WO_3$ at surface densities of 6.4 V and 5.3 W atoms/nm², respectively, as measured by Raman, while IR-based titration of $Ti^{4+}$ surface sites on $TiO_2$ with CO molecules, yielded slightly different values of 5.7 V and 5.2 W atoms/nm². Interestingly, $WO_3$ appears before full surface coverage of $TiO_2$, suggesting early agglomeration, while $V_2O_5$ emerges after complete surface saturation. These findings highlight the necessity of combining both Raman and IR techniques to fully characterize the dispersion of oxides on catalyst surfaces, providing a more accurate understanding of monolayer formation and catalytic behavior.

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# Measurement of composition of natural gas and hydrogen-enriched natural gas mixtures by industrial-grade Raman spectroscopy

The distribution network of natural gas is evolving rapidly toward more complex mixtures, having also hydrogen-enriched compositions. The sector requires for state-of-the-art industrial-grade instrumentation capable to determine the composition and the related quality (in terms of Heating Value) of the gas mixtures distributed in the networks. The gas parameters (mainly the concentration of methane and heavier hydrocarbons, carbon dioxide, nitrogen and hydrogen) need to be monitored in real time and in a wide range of compositions, since mixtures are found within an extremely variable range depending on the origin of the gas.

A compact, fast and highly sensitive instrument based on spontaneous Raman spectroscopy has been developed with the specific aim to operate directly in-line to measure the gas composition within a broad range of gas mixtures and operating temperatures between -20°C and +50°C. This approach is intrinsically non-invasive, since it requires a laser beam passing through the gas cell to excite the Raman emission, and multi-species sensitive, since the different components of the gas mixture are simultaneously detected, particularly species difficult or impossible to be detected with conventional absorption spectroscopy (such as hydrogen and nitrogen).

The Raman scattering is stimulated by a laser diode centered at 455 nm with multi-mode emission and 1.5 W optical power. The laser is focused on a sealed gas cell where the sample gas to be measured is flowing, the Raman emission is collected by a grating spectrometer and finally acquired on a 2D camera. The measured spectra are fitted with the calibration dataset acquired at room temperature to achieve the mixture composition. The system is able to determine the main components of the natural gas: methane, heavier hydrocarbons, nitrogen, carbon dioxide and hydrogen. The Heating Value is finally calculated using the ISO6976:2016 standard.

Several certified gas mixtures have been tested with the instrument operated at different temperatures in the range from -20°C to 50°C, to prove the capability to operate in a wide temperature range, being anyway capable of giving the correct gas composition within the precision required by the measurement standard. The system can operate at pressures variable between 1 and 6 bars, requiring less than 30 s to provide a complete measurement. The system has been validated also with hydrogen-enriched gas mixtures.

Two prototypes are currently being tested in-line in the Italian distribution network and in a biogas production plant.

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# Towards Open, FAIR and Intelligent Raman Spectroscopy

The industrial and academic use of Raman spectroscopy grows in parallel with the need to collect, process, share and reuse digital spectroscopic data efficiently and reliably. Therefore, harmonization and standardization efforts in Raman spectroscopy are essential. In this context, we present:

a) New proposals for Raman instrument calibration and harmonisation, including samples and protocols (CWA 18133:2024 and CWA 18134:2024).
b) The open-source Python package ramanchada2, along with user-friendly, code-free downloadable and web applications, integrating existing and novel state-of-the-art algorithms for generating, reading, and processing Raman spectra, with special emphasis on calibration and algorithm benchmarking    .
c) NeXus data format adapted to Raman spectroscopy to package characterization data with metadata - including processing information- from multiple experiments and even different techniques into a single file using a harmonized structure and terminology.
d) An open source database solution that stores spectra in NeXus format with efficient metadata and spectra search, making it easier to find and compare data from different experiments.

These efforts, part of CHARISMA project (GA952921), pave the way toward FAIR (Findable, Accessible, Interoperable, and Reusable, but also For Artificial Intelligence Readable) Raman data for intelligent processing, which will benefit both private companies and open science. To foster this transformation, stakeholder's engagement and efforts coordination are crucial.

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# Hybrid fs/ps-CARS microscopy for identification of simili-explosive powders

In the past years, intense efforts in Raman based CBRN sensing have been devoted to the detection and identification of trace amounts of hazardous chemicals [1,2] or biological agents [3]. This goal requires high sensitivity as well as the ability to differentiate between compounds very similar in molecular composition but very different in threat. In that purpose, hyperspectral microscopy appears as a very powerful tool since it combines molecular information with morphological details, which are required for precise identification of threat agents, in samples such as bacterial and spores. In this work, hybrid fs/ps-CARS microscopy is applied to the study of nitroaromatic explosives. A spectroscopic study was carried out on two TNT substitutes having very similar chemical formula, namely DNT and DNB, inside their specific spectral windows (symmetrical elongation mode of $NO_2$ at 1350 $cm^{-1}$, C-N bond at 1600 $cm^{-1}$, and C-H bond at 2900 $cm^{-1}$). We show that a single peculiar spectral window, 200 $cm^{-1}$ in width, centered at 1350 $cm^{-1}$ for the $NO_2$ elongation mode, although traditionally known to be intense but lacking of specificity [4], definitely allows for accurate identification of DNT and DNB, thanks to the good spectral resolution (<8 $cm^{-1}$) offered by our hybrid fs/ps-CARS setup. Between 80% and 90% positive identification have indeed been demonstrated using supervised (correlation with reference spectra) or unsupervised (PCA + agglomerative clustering) methods in this single spectral window.

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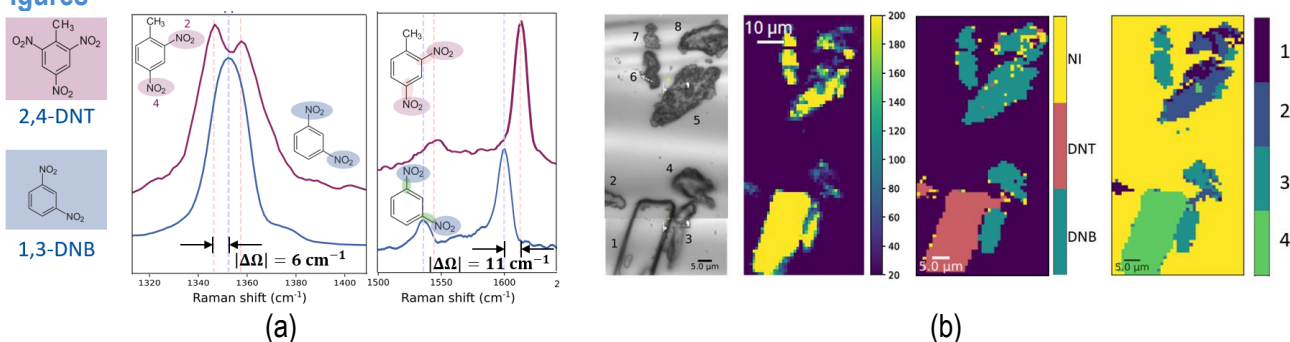[4]  Bremer et al, Proc. SPIE 8358 (CBRNE) Sensing XIII (2012) 835818

## Figures



**Figure 1:** (a) Spectrum of DNT and DNB on the $NO_2$ and CN bounds (b) White light image, CARS image at 1350 cm-1, clustering using supervised and unsupervised method.

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# MiniRaman: Handheld and microscope, for convenient diagnostic assistance.

Miniaturised Raman instruments are helping to develop the handheld and microscope landscape. With handhelds that can fit securely in the palm of one hand, and a microscope adapter that is similar in size to a Bluetooth speaker, the MiniRaman instruments also offer a high sensitivity and resolution in their form factor.

The convenience of testing patients directly in vivo, for example on their skin, can assist in diagnostics and treatments for patients. Skin diagnostics of cancer and atopic dermatitis, is generally considered to require complex Raman instrumentation, especially at 100µm depth.[1,2] The miniRaman has been demonstrated to be able to perform in vivo skin analysis, indicating its future application for skin disease diagnostics.

Fast identification of bacterial strains is important to combat antimicrobial resistance which is increasing worldwide. Using the procedures for sample preparation and data analysis from research that demonstrates a 96% accurate identification model, the miniRaman is shown to be able to compete against the research grade Raman microscope with deep cooled CCD used in the original paper.[3]

Therapeutic drug monitoring (TDM) can be vital for patients undergoing treatments where the drug clearance rate must be monitored to prevent toxic build up or even death. Generally this work is also performed by research grade Raman microscope with deep cooled CCD,[4] which limits the number of instruments that are economic for a hospital to use. The miniRaman is capable of nanopillar-assisted separation (NPAS) method using SERS mapping can be used to measure <75 µM concentration of anti-cancer medication is saline.

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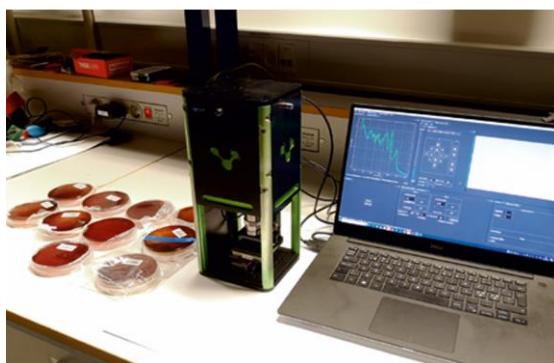


**Figure 1: P**hotograph of miniaturized Raman microscope during Raman mapping of bacteria samples on CaF2 cover glass.

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# Calibration methods for Raman spectrometers in Clinical applications

In order to enable Raman to be widely deployed in clinical practice, the issue of system calibration following production and during clinical use by non-technical users must be addressed. As Raman spectroscopy continues to find new applications in diagnostics, the demand for non-complex and accessible standardisation materials and processes is growing. Despite the availability of numerous standards, there remains significant potential for further development, particularly when driven by specific applications. The lack of viable calibration approaches can be a potential barrier to obtaining regulatory approvals. In this work we have examined multiple materials that can be used for Raman spectra calibration across bench top and portable devices. Since there is a lack in the market for Standard reference materials such as the SRM2241, we propose an alternative: a polymer-based material that can serve as an intensity correction calibration sample for the fingerprint region.

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# Portable Raman Spectrometer – future diagnostic tool in cartilage tissue damage

Alterations in cartilage structure can disrupt joint function and affect tribological properties. These changes can lead to degeneration of joint surfaces and the development of orsteoarthritis, which is a major cause of disability worldwide [1]. Evaluating cartilage degradation in joints is crucial for diagnosing osteoarthritis progression. Although there are diagnostic methods like X-rays and MRI, there are no accurate techniques detecting the early stages of osteoarthrisis.

Raman spectroscopy is emerging as a valuable tool for analyzing tissue surfaces, which could be helpful in establishing the link between the structure of articular cartilage and the progression of degeneration [2]. Previous research indicates that Raman spectroscopy can successfully identify damaged tissues. The versatility of the technique may enable clinical applications. Spectrometer equipped with a probe, could allow for assessment of cartilage degradation during arthroscopy. In this study the human articular cartilage with varying levels of degradation was obtained during joint replacement surgeries from different patients. Preliminary *ex vivo* findings on animal and human cartilage tissue using a fiber-optic Raman probe suggest its potential for diagnosing osteoarthritis.

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# Rapid detection of Pesticide Residues Based on Surface-Enhanced Raman Scattering through Core-Shell nanoparticles

In the context of the rapid development of the food industry and agriculture science and technology, it is very important to detect the target molecules within the complex biological or chemical environment, such as pesticide residues in various foods, pollutant detection in the marine environment, virus detection in vivo, etc. To detect the target molecules with higher sensitivity and linearity, specificity, speed, and reproducibility in a complex environment has always been our pursuit, and quantitative measurement with high accuracy would be another challenge for rapid and accurate trace detection. Recently novel method like surface-enhanced Raman scattering (SERS) has emerged as a promising label-free detection method for multifarious applications due to its advantages of high sensitivity, time-saving experiment process special molecular fingerprint, along with non-destructive nature. Core-shell nanoparticles have been commonly used as surface-enhanced Raman scattering (SERS) substrates for sensing and detection due to their prominent optical properties such as localized surface plasmon resonance (LSPR) and tunability. In this study, AuNRs@Ag core-shell nanoparticles with different thicknesses of silver shells were synthesized. A Raman reporter 1, 4-benzenedithiol (1,4-BDT) was then sandwiched in between the Au-Ag nanogap to obtain a strong Raman signal as a reference signal for the quantitative measurement of the concentration of pesticide residue. The longitudinal resonance peak of AuNRs@Ag core-shell nanoparticles can be tuned from 760 nm to 610 nm by controlling the thickness of the silver shell. Also, we evaluated the SERS-enhancing properties of the AuNRs@1,4-BDT@Ag nanoparticles by measuring the Raman signal of the mixture of these nanoparticles with pesticide residue solutions. The highest detection sensitivity and reproducibility of quantitative measurements were achieved, corresponding to an optimized longitudinal resonance peak and probes. We also combined it with machine learning algorithms to accurately identify and quantify the SERS spectra of the pesticide residue in the system. To evaluate the performance of machine learning algorithms different metrics were applied that demonstrated accuracy in pesticide residue status prediction. This developed approach helps as a simple and expeditious tool for the analysis of food and exhibits potential for broader applications in various domains in the future.

**Figures**
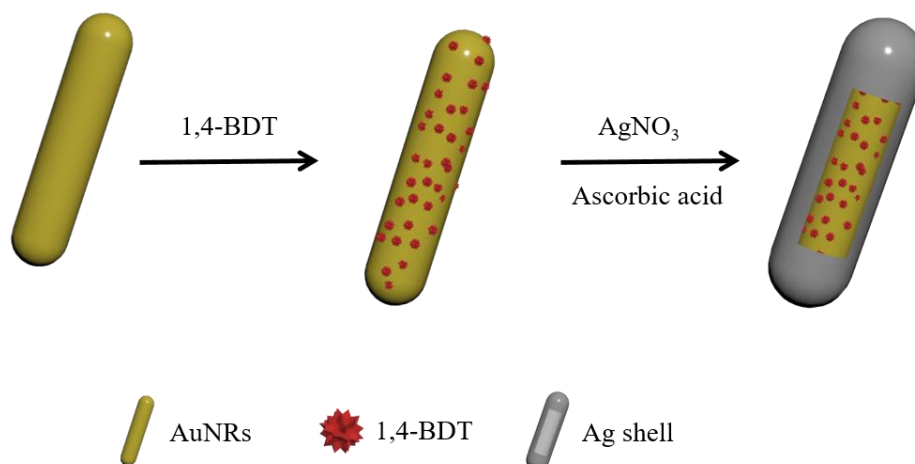


**Figure1.** Schematic fabrication procedure for the core-shell GNRs@1,4-BDT@Ag NPs.

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# Multi-Modal Imaging and Analysis:  Combining Enhanced Darkfield Hyperspectral Microscopy with Confocal Raman Microscopy

Enhanced Darkfield Hyperspectral Microscopy is the preferred imaging and spectral analysis tool for nano-scale biological and materials science applications.  This powerful technique offers rapid visualization, characterization, and mapping of nano-scale entities, as small as 10-20 nm, in a wide range of translucent samples.  Combining this technique with the powerful quantitative analysis offered by confocal Raman provides researchers with a tool of unequaled imaging and spectral analysis capabilities on a single microscope platform.

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# Evaluation of Hyaluronic acid in HA/PVA nanofibers by Raman spectroscopy

Hyaluronic acid (HA) is recently one of the most frequently used materials for the preparation of nanofibers and their subsequent application in the cosmetic industry and medicine. In both fields, its moisturizing, healing effect and quick solubility in water are the biggest benefit [1, 2]. Nanofiber samples of HA mixed with the fiber-forming polymer (Polyvinylalcohol (PVA)) in different ratios were electrospun via 4SPIN LAB® device [1, 3]. The amount of HA, which is contained in nanofibers, is usually evaluated by LC-MS. However, such a method is time consuming, destructive and financially demanding. Therefore, a method for the evaluation of HA by component analysis using Raman spectroscopy was developed. Raman spectroscopy successfully overcomes the mentioned shortcomings of LC-MS and can serve as a comparative technique not only for nanofiber analysis. The results from LC-MS and Raman spectroscopy were compared and it was confirmed that the methods correlate to each other (Tab. 1).

| Sample | HA (wt%) expected | HA (wt% ± SD); Raman | HA (wt% ± SD); LC-MS |
|---|---|---|---|
| HA/PVA_1 | 79,1 | 79,3 ± 1,3 | 79,9 ± 0,5 |
| HA/PVA_2 | 79,1 | 80,7 ± 1,5 | 79,4 ± 1,0 |
| HA/PVA_3 | 60,0 | 59,1 ± 0,6 | 57,8 ± 2,1 |

Table 1 – Results of evaluation of HA in nanofiber samples

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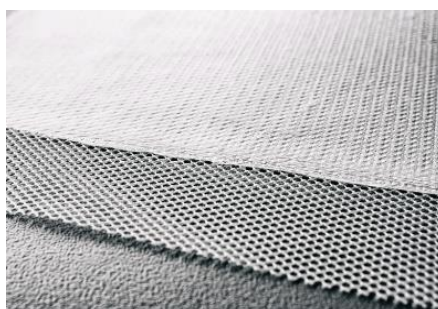
## Figure



**Figure 1:** HA/PVA nanofibers electrospun onto substrate

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# Correlative techniques to probe micro- and nanoparticles and their human health implications

The presence of micro- and nanoparticles in the world has notably increased in recent years, especially those related to cosmetics products and plastic materials. Several scientific publications study the impact of such particle size range on human health [1,2]. A single technique cannot provide a full characterization of the particle, nor a complete understanding of its impact on humans. Multiple correlative techniques are required for a comprehensive analysis of the particles, which can vary in size, shape, and composition. This study outlines an investigation into the detection, characterization, and spatial mapping of these particles, emphasizing their presence in water sources and cosmetic products. Microplastics coming from water sources are considered a primary human exposure pathway, becoming crucial to be analyzed, characterized, and identified as an important vector of human contamination. Cosmetics are composed of a complex mixture of components, including micro- and nanoparticles that, in contact with the skin surface, can easily penetrate and play a key role in the body, either by protecting the skin or affecting essential mechanisms. Both cases deal with complex matrices and deserve the combination of several techniques. Correlating Atomic Force Microscopy (AFM), which facilitates high resolution imaging, enabling the visualization of surface morphology, mechanical properties, and spatial distribution of nanoparticles, and Raman spectroscopy, which discerns molecular composition, structural integrity, and chemical interactions, providing insights into the identity and behavior of nanoparticles, we were able to fully characterize these particles down to the nanoscale, gaining insights into their morphology, chemical composition, and distribution. A key aspect of our study involves the application of nanoGPS technology, facilitating data correlation across diverse microscopy techniques. This method enables precise spatial localization of particles, allowing comprehensive integration of information from various analytical methods. Our findings underscore the necessity for advanced analytical techniques in assessing health risks associated with micro and nanoparticle exposure.

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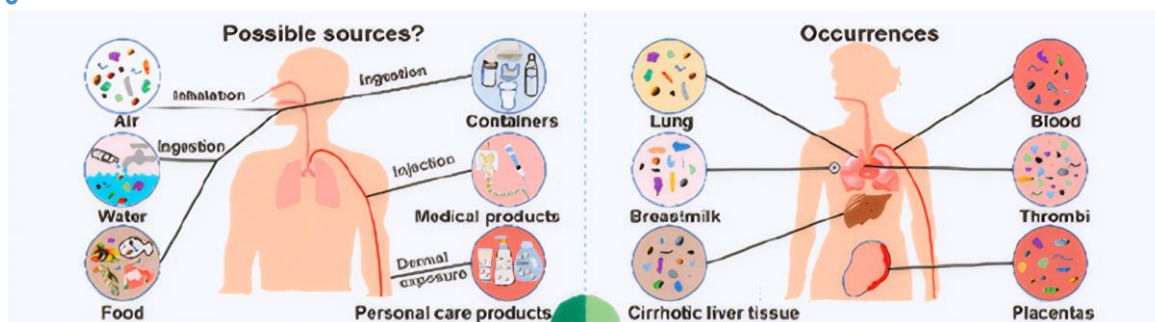
## Figure



**Figure 1:** Possible sources and occurrences of micro and nano plastics in the human body. [1]

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# Hyperspectral unmixing for Raman spectroscopy via physics-constrained autoencoders

Raman spectroscopy is widely used across scientific domains to characterize the chemical composition of samples in a nondestructive, label-free manner. Many applications entail the unmixing of signals from mixtures of molecular species to identify the individual components present and their proportions, yet conventional methods for chemometrics often struggle with complex mixture scenarios encountered in practice. Here, we develop hyperspectral unmixing algorithms based on autoencoder neural networks, and we systematically validate them using both synthetic and experimental benchmark datasets created in-house. Our results demonstrate that unmixing autoencoders provide improved accuracy, robustness, and efficiency compared to standard unmixing methods. We also showcase the applicability of autoencoders to complex biological settings by showing improved biochemical characterization of volumetric Raman imaging data from a monocytic THP-1 cell (Figure 1).
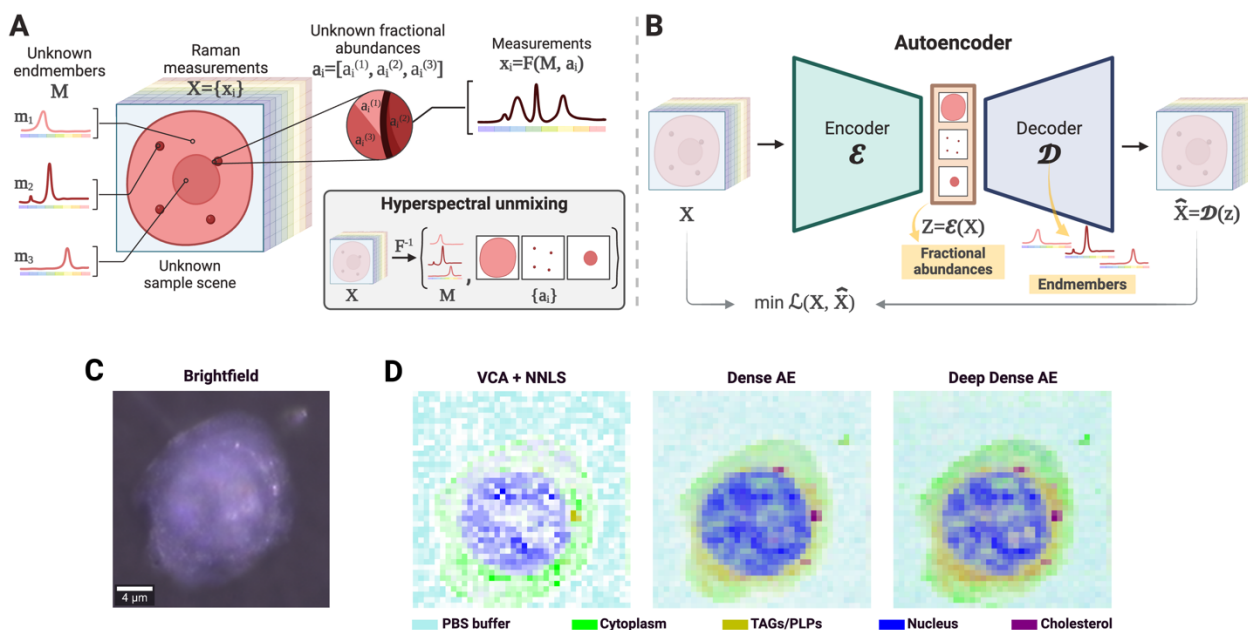


**Figure 1:** Improved Raman cell imaging via Raman unmixing autoencoders. (A) Illustration of cell imaging via hyperspectral unmixing. (B) Hyperspectral unmixing as a self-supervised autoencoder learning problem. (C) Brightfield image of the studied THP-1 cell (data from Kallepitis et al. (2017) [1]). (D) Image reconstructions of the cell obtained by: a standard method for unmixing - VCA [2] + NNLS [3]; our dense autoencoder model; and a deeper version of our dense autoencoder.

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# Mineralogical and copper isotopic characteristics of various types of native copper mineralization

Micro-Raman spectroscopy was used to identify mineral species in various types of native copper deposits from Japan. Five reference products of clay minerals, including kaolinite (JCSS1101b), dickite (JCSS1301), pyrophyllite (JCSS2101), montmorillonite (JCSS3101), and saponite (JCSS3501) were also analyzed to optimize analytical conditions and to obtain reference spectra of clay minerals [1]. Primary chalcopyrite, secondary copper-bearing minerals (cuprite, malachite, and langite), and montmorillonite were identified with Raman analyses of supergene native copper. Magmatic native copper occurs in fresh olivine from an orogenic peridotite massif [2]. Micro-Raman measurements indicated that there were no serpentine and clay minerals around the native copper. In contrast, micro-Raman results revealed that native copper from serpentinized peridotite was associated with primary pentlandite and secondary malachite, oxide minerals, and carbonate minerals. The copper isotopic values ($\delta^{65}Cu$ = [($^{65}Cu/^{63}Cu)_{sample}$/ $(^{65}Cu/^{63}Cu)_{NIST-SRM976}$-1] × 1000) of the supergene native copper ($\delta^{65}Cu$ = 1.4 to 1.7‰ [3]) and the associated secondary copper-bearing minerals ($\delta^{65}Cu$ = 2.2−3.1‰) were significantly heavier than those of the primary chalcopyrite (−0.3 to 0.2‰) from the same deposit. Copper isotopic ratios of the magmatic native copper are in a relatively narrow range (0.0 to 0.1‰) [2]. The native copper from the serpentinized peridotite had negative $\delta^{65}Cu$ values (-0.7 to -0.4‰), whereas the associated secondary malachite had positive $\delta^{65}Cu$ values (1.0 to 1.2‰). There were significant differences in $\delta^{65}Cu$ values between native copper and associated copper-bearing minerals. Therefore, pre-identification of minerals associated with native copper using micro-Raman spectroscopy is important to understand intrinsic isotopic signatures of these samples.

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# Fatty acid composition prediction and phenomic selection in rainbow trout by Raman spectroscopy

In this study, Raman scattering spectroscopy was used to predict fatty acid (FA) composition in rainbow trout (Oncorhynchus mykiss), providing a cost-effective alternative to gas chromatography (GC). Fatty acid composition was analysed in visceral adipose tissue from 268 individuals fed three different diets. Ridge regression was used to calibrate a model against GC results. The FA profile of 1,382 trout from 831 families of the "Les Sources de l'Avance" selection programme was then predicted from Raman spectra obtained from visceral fat sample, and phenotypic data for growth, processing and quality traits, including a cross-sectional steak image using magnetic resonance imaging, were also collected. A 57k Axiom™ single nucleotide polymorphism genotyping array was also used to provide heritability (h2) estimates along wavenumbers. Heritability is the proportion of observed variation in a trait among individuals in a population that can be attributed to genetic factors, indicating how much a trait is likely to be passed from parents to offspring.

The results yielded cross-validated R² values of 0.79 for total PUFAs, 0.83 for omega-6 PUFAs and 0.66 for omega-3 PUFAs. Individual omega-3 fatty acids such as alpha-linolenic acid (ALA), eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA) also showed strong predictive performance with R² values of 0.82, 0.76 and 0.81 respectively. The heritability results show that the Raman spectra are significantly heritable with three interesting wavenumbers (h2 from 0.15 to 0.28). Phenomic selection showed higher correlations with corrected phenotypes for traits such as body weight and fatty acid composition, outperforming genomic selection in these cases. Further validation in future generations will be required to confirm these findings.

Taken together, these results demonstrate the potential of the Raman spectroscopy and multivariate statistics principle to improve aquaculture breeding programmes by integrating high-throughput FA composition prediction by Raman spectroscopy and phenomic selection to support more efficient large-scale phenotyping [1,2].

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# Innovative Raman Measurement Technique with a Uniform Line Focus for LFT readout

Several spectroscopic methods are available for reading the test and control lines of Lateral Flow Tests (LFTs). Raman spectroscopy stands out due to its ability to provide distinct molecular bands, clearly separated from the background spectrum. This characteristic allows for more reliable identification of markers at the test and control lines, resulting in tests that are both more specific and sensitive, offering improved quantification of analytes [1]. Although pure Raman scattering suffers from a low quantum yield, this limitation can be overcome by using marker particles that enhance the Raman scattering cross-section via plasmonic effects, a technique known as Surface Enhanced Raman Spectroscopy (SERS). SERS enables ultrasensitive and rapid quantification of analytes, such as viral particles, even in complex environmental samples [2].

However, a key challenge in Raman spectroscopy is balancing maximum quantum yield with the risk of thermal damage to the LFT. To mitigate this risk, it is preferable to use a line focus rather than a conventional point focus for the excitation laser. This can be achieved using a cylindrical lens to form the line focus. Yet, even without further beam shaping, there tends to be a peak in intensity at the center of the line. This study aimed to develop a Raman measurement technique that produces a uniform line focus, enabling non-destructive analysis of LFTs without causing thermal damage or overheating. Two approaches were explored: the first involved using a beam-shaping lens, which delivered stable and reproducible measurements but required additional optical components and increased the distance between the Raman probe and the sample, leading to significant signal attenuation. The second approach utilized a rectangular fiber in conjunction with a cylindrical lens to produce a uniform line focus, resulting in a homogeneous output beam without the need for additional optical elements. This novel solution proved to be the more effective method. Here, we present our findings based on newly developed multiplex LFTs for veterinary applications.

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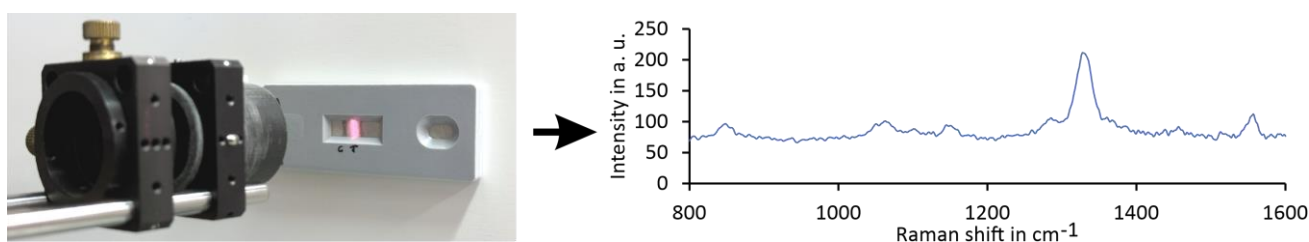
## Figures



**Figure 1:** Creating a uniform line focus using a rectangle fiber to generate Rama spectra of the test and control line.

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# Microplastics analysis in food: assessing human exposure through Raman micro-spectroscopy

Microplastics are small particles of synthetic polymers, insoluble in water, ranging in size from 1 µm to 5 mm. They have been detected in various environmental matrices,in drinking water and food [1], and are now recognized as emerging particulate anthropogenic pollutants. Due to their persistent nature and potential harmful effects on both human health and the environment, microplastics have become a growing concern.

Current efforts by the scientific community and standardization bodies are focused on assessing the risks associated with microplastics exposure. These initiatives aim to gather comprehensive data on real-world exposure levels and to evaluate the impacts of microplastics on living organisms.

Raman micro-spectroscopy is recognized as a reference method for monitoring microplastics, allowing for chemical identification, particle size measurement, and particle quantification [2].

In this work, a standardized analytical protocol for microplastics detection was applied to a sugar sample. Rapid, automated analysis of thousands of particles down to 5 µm in size was carried out using Particle Finder™ and ID Finder™ software. The results revealed an alarming number of microplastic particles smaller than 20 µm in diameter.

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# Blue, naturally aged polypropylene in aquatic environment as a SERS label: prospect for AgNPs adsorption and its complexes

Detecting and characterizing microplastic particles with normal Raman spectroscopy is usual practice for environmental water samples [1,2]. The possibility of SERS as a tool to detect nanoplastics [3] inspired us to synthesize micro- and nanoplastic particles (MNPs) derived from years-aged blue polypropylene plastic (PP), coated with silver nanoparticles (AgNPs) from a modified Lee-Meisel procedure [4]. We aim to elucidate the interaction between AgNPs and blue PP MNPs, and to draw conclusions on the influence of the blue pigment (PB15) incorporated in plastic in the overall SERS capability to detect and quantify nanoplastic in environmental waters. In addition, X-ray diffraction was used to check the aged PP crystallinity and correlate it with plastic age and pigment integrity. Characterization of the AgNP colloid obtained in the presence of MNPs plastics was performed with UV-Vis and SEM/TEM. The evaluation of the PB-15 persistence in MNPs PP was done with resonance Raman spectroscopy to selectively detect the PB15 in <µm size particles inside AgNP colloid solution, as well as the bulk normal Raman spectroscopy of AgNP colloid containing plastics. Further validation of persistence of the pigment is evaluated via drop coated Raman deposition (DCDR). Plastics coated with AgNP were evaluated for SERS enhancement using crystal violet (CV) and methylene blue (MB) as test molecules for µM concentrations, revealing unaltered enhancement compared to the classical AgNPs. Thus, the approach allowed improved capability of SERS for blue, environmentally abundant nanoplastic screening.

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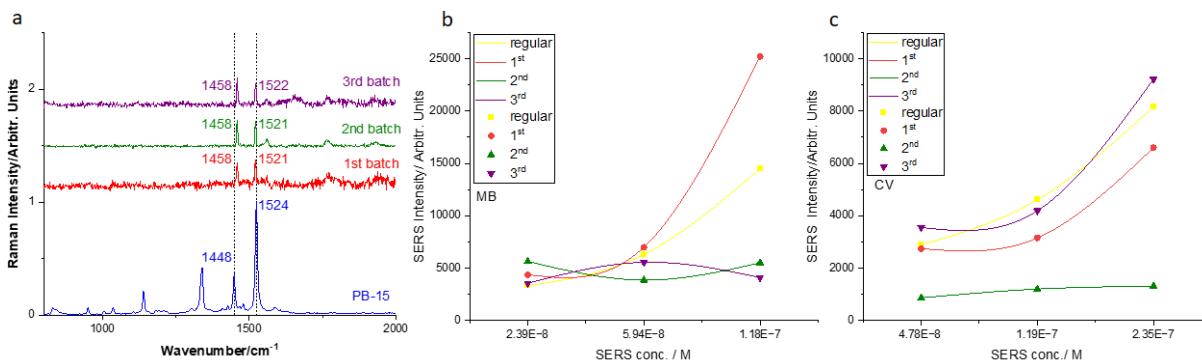[4] P.C. Lee et D. Meisel, J. Phys. Chem. (1982), 86, 3391–3395.

## Figures



Figure 1: a) PB-15 persistence in AgNP colloid, SERS absolute intensity as a function of the SERS concentration of the analyte b)CV c) MB

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# Surface property studies on modified $VO_x$/$TiO_2$ catalysts for the $NO_x$ abatement in mobile sources

Emissions of nitrogen oxide gases ($NO_x$) originating from combustion processes attract significant attention due to their role as a major source of atmospheric contamination, along with health risks and a series of environmental issues.[1] Since combustion processes in mobile sources (e.g. heavy-duty vehicles such as trucks or ships) are expected to be used for a foreseeable future, many efforts have been invested in the development of suitable de$NO_x$ technologies. The selective catalytic reduction with ammonia ($NH_3$-SCR) is one of the most established technologies, where the formed $NO_x$ gases are catalytically converted into harmless nitrogen and water. Vanadium oxide-based ($VO_x$) catalysts are one of the most commonly used catalyst types given to the low material costs and high chemical resistance (such as sulfuric compounds).[2] However, the application in mobile sources provokes several challenges, as the catalyst has to work under dynamic conditions in a broad temperature window. Both low-temperature activity and stability at high temperatures are required.[3] Since the operation temperature in automobiles varies between ambient and maximum temperature, the effects of temperature and time, are weighted together in a defined aging procedure considered representative of the application at hand.[4] Promising solutions have emerged with the modification by metal oxides to stabilize both the active vanadium oxides as well as the $TiO_2$ support.

For a rational design of a new generation of $NH_3$-SCR catalysts, a scientific understanding of the fundamental limitations for catalyst activity, selectivity and stability must be achieved. Our work will present systematic studies of the surface properties on modified $VO_x$/$TiO_2$ catalyst in terms of structure, the interaction between the support and additives as well additives and vanadium with the aid of various *ex situ* characterization techniques such as $N_2$-physisorption, temperature programmed desorption, XRD. In addition, the catalysts were thermally treated to mimic a long-term use and to study the respective impact. Infrared spectroscopic methods such as Raman and *in situ* DRIFTS allow the identification of surface vanadium oxide species and band assignments for the surface hydroxyl groups along with the formation of adsorbed surface species of the main reactants ($NH_3$, NO). The deconvolution of the $NO_x$ adsorption spectra gives insights to the distribution of the surface species among the samples.

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# Let's go further in materials characterization thanks to co-localization of Raman and μ-XRF analysis

Abstract:

Correlated measurements between microscopy techniques is always challenging and mandatory. Matching molecular mappings with elemental mappings will bring a sum of valuable information for research or industrial applications.

Raman microscopy and MicroXRF can extract both spectrum and mapping information.

We will then present benefits and how HORIBA is handling its internal solution to correlate molecular and elemental analysis through two applications: minerals and pharmaceuticals, spectra and mappings.

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# Raman Spectroscopy Tools for Quality Assessment and Sustainable Pigments Extraction from Shrimp Tissues

Bioeconomy plays an important role in the current research fields with crustacean waste valorization being one of the most extensively investigated topics. In this regard, many studies have been conducted on crustacean waste, identifying astaxanthin as the primary pigment found in crustaceans [1,2]. The monitoring of carotenoid profile in the shrimp tissues [3], along with the characterization of the extracts is not yet fully explored.

This study applies Resonant Raman Spectroscopy to evaluate the efficacy of an eco-friendly pigment extraction method on shrimp soft and hard tissues. Acetic acid was used as the extraction agent. Spectroscopic analysis revealed notable pigment extraction in the acidic bath solution, as confirmed through Surface-Enhanced Raman Spectroscopy (SERS) measurements of the extract solutions. The Resonant Raman spectra revealed significant reduction in the carotenoid profile of the shrimp tissues after 12 hours of acetic acid immersion. These findings support the use of mild acids to selectively isolate bioactive compounds while preserving structural integrity, which is consistent with recent research on environmentally friendly extraction techniques in marine biomaterials [4].

Our study highlights Resonant Raman Spectroscopy and SERS as effective tools for tracking pigment extraction, offering insights into sustainable approaches for bioresource valorization in seafood processing.

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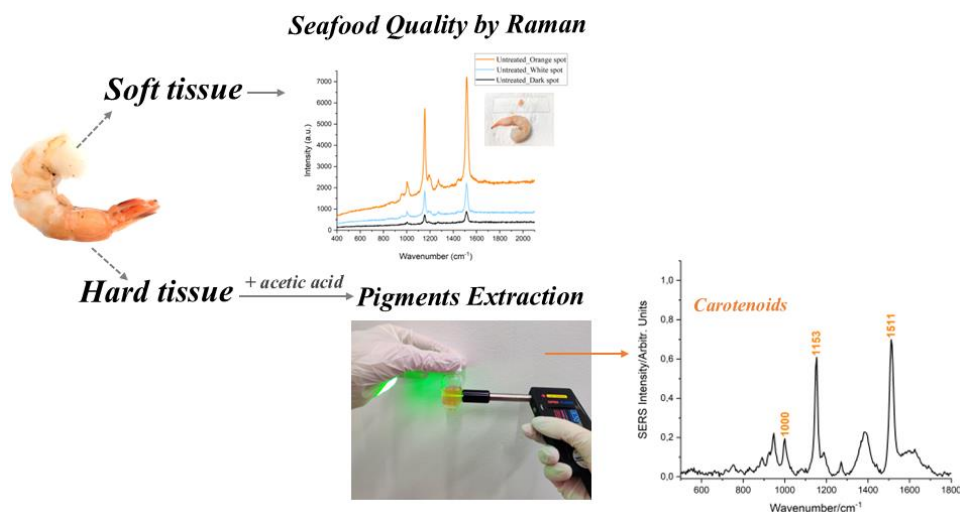[4]  A. K. Wani et al., Environ. Sci. Pollut. Res. Int., 31:38960–38989 (2024)

## Figures



**Figure 1:** Raman Spectroscopy tools for quality assessment and pigment profiling in shrimp tissues

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# IDFinder: The HORIBA Solution for Spectral Identification

IDFinder offers one-click instant identification for single and multi-component searches, identifying materials from Raman spectra. Integrated into all LabSpec 6 modules, IDFinder enhances workflows such as MVA+ for detailed multivariate analysis, ParticleFinder for high-throughput particle identification, and Layers for characterizing multilayer structures. Illustrated through pharmaceutical tablet analysis, particle detection, and multilayer materials, IDFinder provides unmatched flexibility and precision. With an intuitive interface and extensive library management, it transforms spectral identification for diverse research and industrial applications.

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# Using Raman Mapping with FIB and SEM to characterize complex 3D structures in PEM electrolyzer materials

Proton exchange membrane (PEM) electrolyzers are part of a cohort of technologies that promise to enable a green and scalable energy system based upon hydrogen. Central to their operation is the membrane electrode assembly (MEA), consisting of two electrodes and a membrane. Here there is a large materials science challenge as the MEA needs to provide good electrical contact, catalyst access, mass transport processes in aqueous and gaseous phase, and high durability in a harsh electrochemical environment [2]. To develop such materials, it is vital to understand both their morphological and chemical properties, however this is often challenging due to the 3-dimensional differences in the materials and the difficulty in accessing different sections of a material with most instruments. The Pt-covered carbon nanofiber anodes produced by Smoltek AB exemplify this, as there are major differences in eg. the void fraction, distribution of supporting ionomer and distance to the membrane at different parts of the material. By using a focused ion beam (FIB) to make a diagonal section into the material, the depth of the material can be explored using SEM to track morphology and Raman spectroscopy to track characteristic chemical bonds, such as the Iridium oxide catalyst [3].

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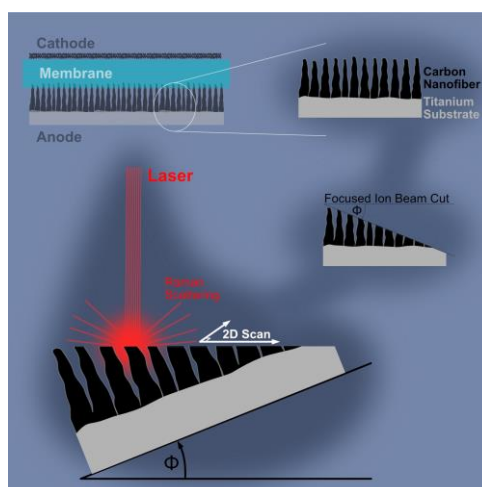[3]  Zoran Pavlovic et. Al., Chem. Commun., 53 (2017) 12414-12417

## Figures



**Figure 1:** Schematic process for using a diagonal FIB section to enable better Raman mapping of a 3D electrode structure

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# Beyond Traditional Methods: Raman Spectroscopy for Breast Cancer Characterization

Raman spectroscopy is a promising investigative and diagnostic tool, which provides information about the molecular structure of a sample. Given the distinct molecular composition of each sample, the spectroscopic profile derived from Raman-active functional groups found in nucleic acids, proteins, lipids, and carbohydrates enables the categorization and differentiation of tissues or cell lines [1].

In this study, we aimed to differentiate between two HER-2 overexpressing breast cancer cell lines, JIMT-1 and SKBR-3, solely based on their Raman spectra. The key difference between JIMT-1 and SKBR-3 cells lies in their response to HER2-targeted therapies (trastuzumab), with JIMT-1 cells being resistant to the treatment, while SKBR-3 cells typically exhibit a favorable response [2].

To collect raman spectroscopic data from single cells, we used a spectro-microscope (LabRAM HR Evolution, Horiba Scientific), with 20x objective, 532nm excitation laser. Instead of using regular culture plate, the cells were seeded on special silica plates to optimize signal-noise ratio, as silica has a distinct raman peak at ~530nm, but is otherwise inert to Raman scattering. Preprocessing of the data was carried out before the analysis using custom software, which included baseline correction, vector normalization, and Savitzky-Golay smoothing.

We successfully developed the methodology required to carry out high-quality Raman spectro-microscopic measurements of single cells, using silica plates and special plating technique, resulting in significant reduction in background noise. We developed a custom, reusable data preprocessing software, to extract the relevant data from the measurements. The classification of the cell lines based on the first and second principal components using a support vector machine (SVM) achieved high accuracy, with a ROC-AUC of approximately 0.9.

Raman spectroscopy being non-invasive and label-free, may offer rapid molecular analysis of cells or tissues both in-vivo or in-vitro. There are several potential applications where the method can potentially be used, including in-situ biopsy assessment, cancer diagnosis, or laboratory analysis.

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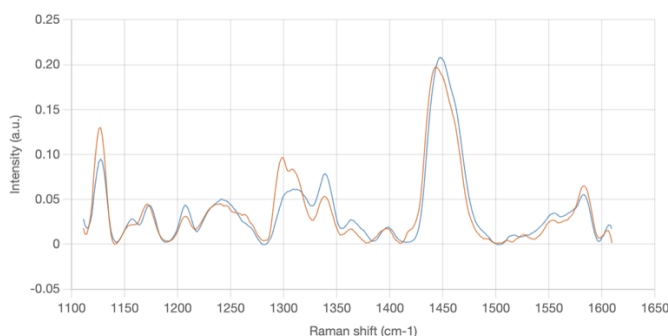
## Figures



**Figure 1**: Raman spectra of JIMT-1 (blue) and SKBR-3 (orange) cells.

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# Raman imaging of MoOₓ nanoparticles – characterization, cell internalization and comparison with s-SNOM imaging

Raman spectroscopy imaging has emerged as a potent tool for localizing nanostructures in cells and identifying their subcellular environment [1]. In our recent work, we prepared photothermal $MoO_X$ nanoparticles through multiple preparation routes (liquid-phase exfoliation [2], microwave-assisted synthesis [3]) and investigated their properties related to the typical oxygen-defect structure and their biocompatibility [2]. In this contribution, we explore Confocal Raman Microscopy (CRM) of $MoO_X$ nanoparticles in fixed cell samples and compare it to s-SNOM image (scanning Scattering Near Optical Microscopy). We evaluate both methods side by side in terms of the information provided, measurement features, and their ability to resolve cell structures as well as internalized $MoO_X$ nanoparticles. Both techniques enable single-cell imaging, nanoparticle localization in cell compartments and provide the ability of tracking physicochemical changes of nanoparticles after their internalization.

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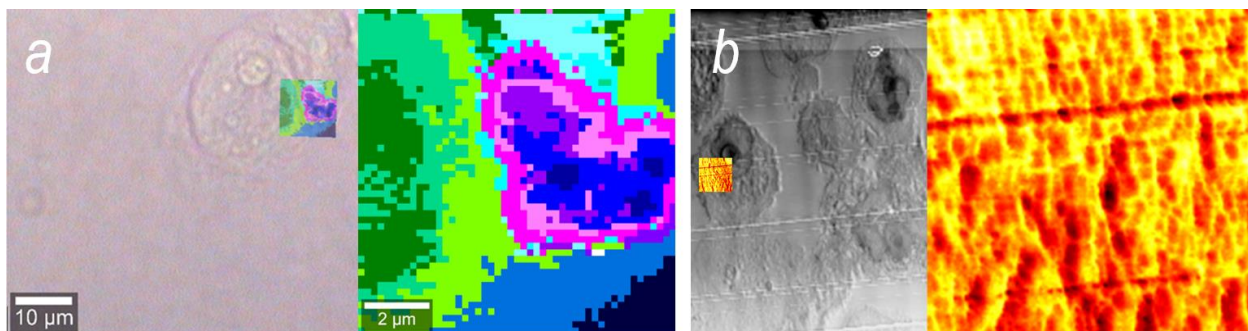
## Figures



**Figure 1:** CRM image (*a*) and s-SNOM image (*b*) of $MoO_X$ nanoparticles in fixed cells. (a) Pink and violet shades internalized $MoO_X$. (b) AFM mechanical scan is complemented by the $MoO_X$ optical amplitude s-SNOM signal at 1050 rel. $cm^{-1}$ (darker means higher intensity).

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## Evidence for Cu-O chain breaking in ion-irradiated high temperature superconductors for magnetic confinement fusion

Compact tokamak concepts, to achieve magnetically confined nuclear fusion, are facilitated by the use of rare-earth barium copper oxide (REBCO) superconducting coated conductors (CC) for their magnets. REBCO offers a comparatively high transition temperature ($T_c$), upper critical field ($B_{c2}$), and current carrying ability in high fields relative to conventional $Nb_3Sn$ or Nb-Ti [1]. However, a drawback of compact tokamak designs is the reduced space available for neutron shielding, exposing the magnets to larger high-energy neutron and gamma fluxes than in less compact reactor designs [2]. Radiation damage produces a combination of nanometre cascades and point defects, particularly in the Cu-O chain anion sites [3], [4]. This leads to a degradation in the critical parameters of the materials and consequently its performance [5]. Raman spectroscopy is an underutilized method to investigate the local disorder in irradiated REBCO. Historical experimental and ab-initio computational work on thin films and bulks has proven the effectiveness in identifying the characteristic REBCO modes, as well as specific defects and impurity phases [6], [7], [8].

Irradiation damage in REBCO primarily produces two types of oxygen sub-lattice damage: displacement of oxygen from the O1 chain site [9], [10], and formation of Frenkel pairs in the $CuO_2$ planes [11]. In this work, evidence for the irradiation-induced breaking of Cu1-O1 chains in REBCO is shown for the first-time using Raman spectroscopy. Experimental Raman spectra of pristine 2 MeV $He^+$ ion-proxy irradiated samples from commercial CC manufacturers are presented, and modelling with the ab-initio density-functional theory code CASTEP is used to identify the modes. Additional spectra of lab-grown pulsed laser deposition REBCO thin films are presented in their pristine state, following a 300 keV $He^+$ ion irradiation to damage levels that completely suppressed superconductivity, and following a post-irradiation oxygen anneal. The spectra changed significantly by broadening, hardening, and softening of specific peaks. Most interestingly, the oxygen sublattice is seen to change during this process, showing an increase in the relative intensity of the Cu1-O1 chain mode following irradiation, indicating a breaking of the Cu-O chains, which are essential to the transfer of superconducting charge carriers to the $CuO_2$ superconducting planes. A 24-hour $O_2$ anneal appeared to replenish the oxygen in the chains, indicated by the disappearance of the defect chain modes. Meanwhile the cation lattice appears unchanged following the anneal. This work supports previous studies that show the displacement of O1 site oxygens to be a key factor in the degradation of superconducting performance.

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# Towards the Analysis of Nanoplastics Using Sub-Micron Optical-Photothermal Infrared (O-PTIR) and Simultaneous Raman Microspectroscopy

The widespread use of plastic materials has led to the global presence of microplastics (1 µm to 1 mm) and nanoplastics (<1 µm) in the environment and consumer products. The risks posed by these particles depend on their type, morphology, and size, with nanoplastics being particularly hazardous due to their ability to penetrate biological barriers and transport absorbed toxic compounds, facilitated by their small size and large surface-to-volume ratio [1]. This highlights the need for advanced detection methods for nanoplastics.

Traditional Fourier-transform infrared (FTIR) spectroscopy can only detect particles larger than ~10 µm, while Raman spectroscopy can identify particles down to 1 µm, and sometimes even 300-500 nm, but often suffers from fluorescence interference [2].

Optical-Photothermal Infrared Spectroscopy (O-PTIR) is a novel technique that addresses these limitations. By combining the high spatial resolution of Raman spectroscopy with the chemical specificity of infrared (IR) spectroscopy, O-PTIR achieves IR spectra at submicron spatial resolution, which is particularly beneficial for analyzing nanoplastics affected by fluorescence interference.
Additionally, O-PTIR allows for the simultaneous collection of IR and Raman spectra, providing complementary information and cross-validation between these techniques. This dual-spectroscopy approach enhances the accuracy and reliability of nanoplastic detection and characterization.

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# FT-Raman spectroscopy for authentication of olives from 11 different cultivars in Andalusia, Spain.

Abstract

Using an affordable spectroscopic technique and based on the characteristics of the whole olive stone, the Raman spectral fingerprint associated with molecular differences among 11 of the most common olive varieties in Andalusian groves has been obtained (figure 1). Microstructural analysis, combined with statistical evaluation, allows the detection of indicators that uniquely identify each olive variety without requiring the full spectrum; only a few components from a simple spectrum of the olive stone are necessary. The main goal of this study is to identify and classify olives by variety, either at the initial stages of olive oil production or from microscopic residues in finished products. This approach aims to provide a quality control tool within the oil production chain to verify olive variety.
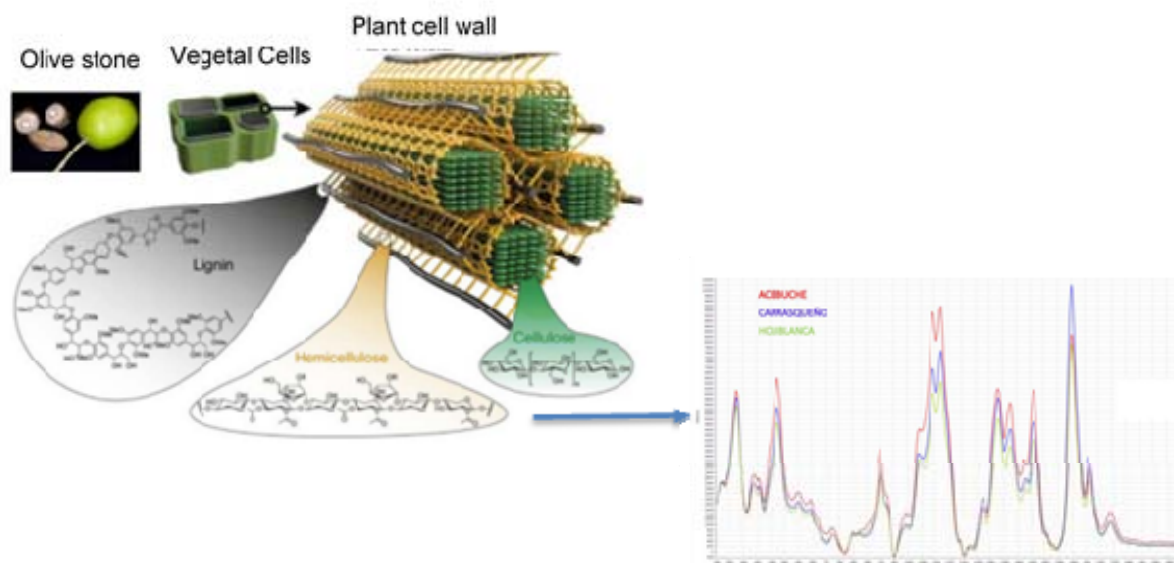
**Figure 1:** Main components of olive stones, including hemicellulose, cellulose, and lignin, along with their composition in proteins, fats, phenols, free sugars, and polyols and Raman spectral characteristics of olive stones in the 200-2000 cm⁻¹ range for the Acebuche, Hojiblanca, and Carrasqueño varieties.

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# Micro-Raman analysis of ancient silver coins: digging into composition, corrosion products and surface morphology.

Silver coins are valuable archaeological objects as they inform precisely on the period, economic relations and even political events from the site they were found. Their material study helps distinguishing between several ores that may have been used and can reveal possible alloys or production processes[1]. However, ancient silver coins can show various corrosion products on their surface which limits non-invasive analysis[2]. Recent publications have allowed a better understanding and identification or silver corrosion products with the use of Raman spectroscopy[3]. Here, one silver tetradrachm minted in the name of Alexander the Great has been studied using micro-Raman spectroscopy. Several corrosion products have been found, as well as impurities and morphological elements revealing recent handling and restoration treatments. This preliminary work aims to better understand the patina of antique coins for upcoming multi-instrumental surface analysis of a large corpus.

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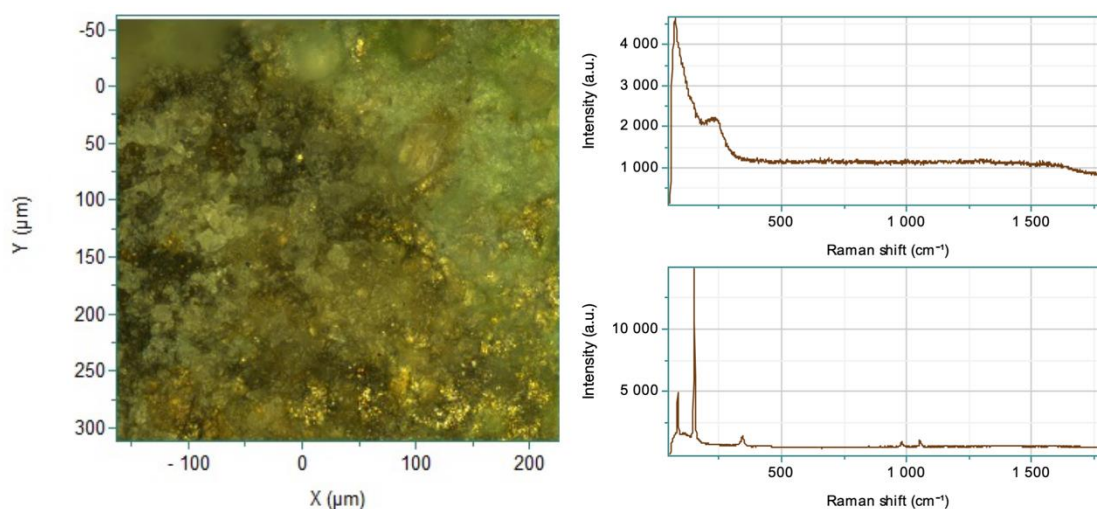
## Figures



**Figure 1:** Microscope image of the surface of the silver coin and selected spectra.