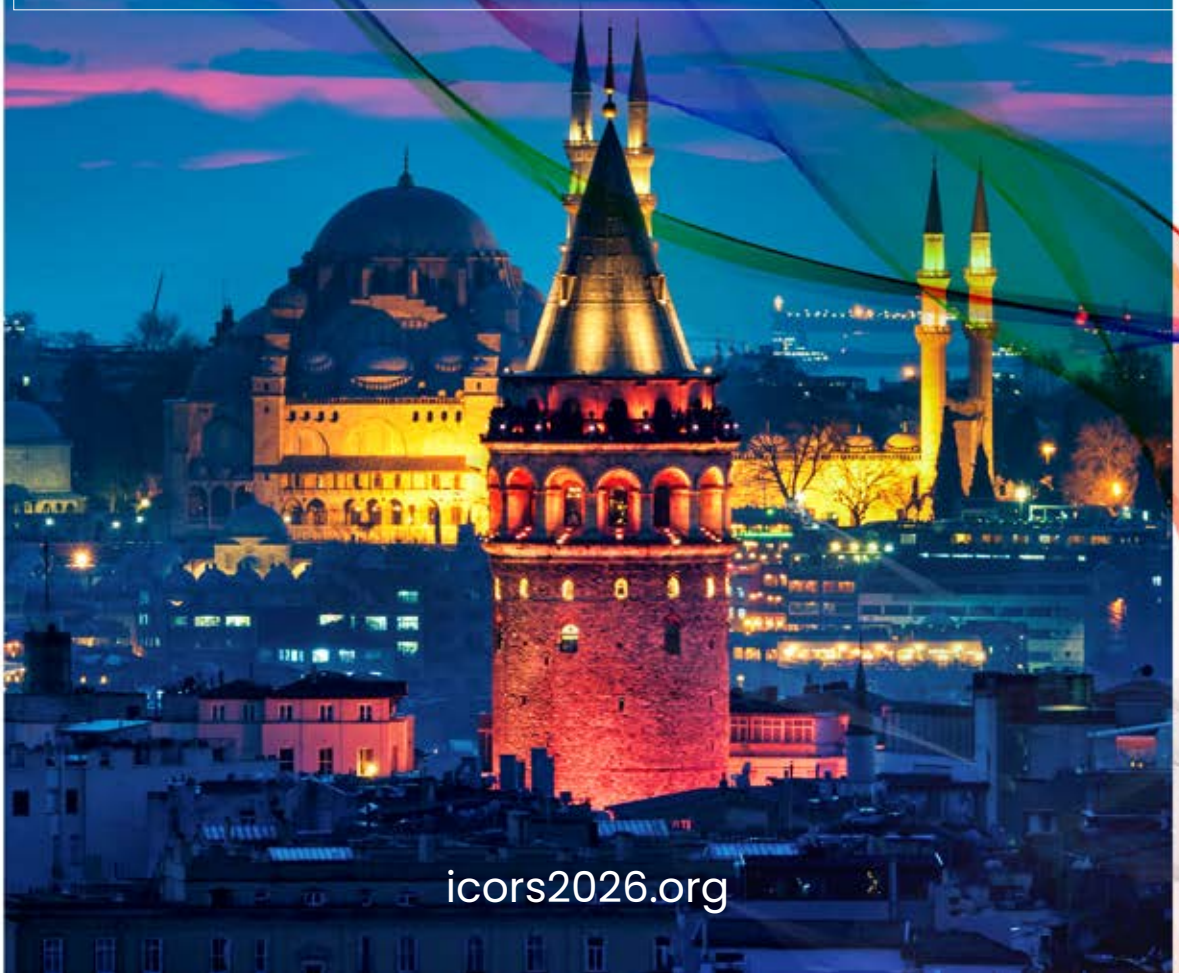
XXIX ICORS

29th International Conference on Raman Spectroscopy

Istanbul TÜRKİYE

23–27 August 2026

BOOK OF ABSTRACTS



icors2026.org

BOOK OF ABSTRACTS

CONTENTS

COMMITTEES	2
SCIENTIFIC PROGRAMME	4
PLENARY LECTURES	20
KEYNOTE LECTURES	29
INVITED LECTURES	48
ORAL ABSTRACTS	72
POSTER ABSTRACTS	356

COMMITTEES

Organizing Committee

Prof. Dr. Mustafa Culha
Conference Chair

Elif Ozturk Er
Istanbul Technical University

Elif Genceli Güner
Istanbul Technical University

Gamze Nese Ozcan
Istanbul Technical University

Caner Unlu
Istanbul Technical University

Ilgin Nar
Istanbul Technical University

Mehmet Kahraman
Gaziantep University

Ugur Tamer
Gazi University

Ismail Hakki Boyaci
Hacettepe University

Mine Altunbek

COMMITTEES

International Steering Committee

V. Ara Apkarian *(USA)*
Sanford Asher *(USA)*
Chiara Cappelli *(Italy)*
Paul Champion *(USA)*
Marc Cicerone *(USA)*
Volker Deckert *(Germany)*
Karen Faulds *(UK)*
Hiro-o Hamaguchi *(Taiwan)*
Young Mee Jung *(South Korea)*
Dongho Kim *(South Korea)*
Janina Kneipp *(Germany)*
Wei Min *(USA)*
Jürgen Popp *(Germany)*
Yuika Saito *(Japan)*
Tullio Scopigno *(Italy)*
Ping-Heng Tan *(China)*
Siva Umapathy *(India)*
Angela Hight Walker *(USA)*
SL Zhang *(China)*
Dalva Lúcia Araújo de Faria *(Brazil)*
Natalie Belsey *(UK)*
Giulio Cerullo *(Italy)*
Chia-Liang Cheng *(Taiwan)*
Mustafa Culha *(Turkey)*
Laura Fabris *(Italy)*
Peter Fredericks *(Australia)*
Koichi Iwata *(Japan)*
Wolfgang Kiefer *(Germany)*
Judy Kim *(USA)*
Jianfeng Li *(China)*
Janos Mink *(Hungary)*
Eric Potma *(USA)*
Sebastian Schlücker *(Germany)*
Antonio G. Souza Filho *(Brazil)*
Zhongqun Tian *(China)*
Yuling Wang *(Australia)*
Nai-Teng Yu *(China)*
Lawrence Ziegler *(USA)*
Prof. Dae Hong Jeong *(South Korea)*

Scientific Programme

23 August 2026, Sunday

	HALL 1 - AMPHITHEATER
09:30-16:00	Registration
17:00- 17:30	**Opening Ceremony**
17:30- 18:15	**Plenary: Prof. Renato Zenobi** *(ETH Zurich, Switzerland)* "TERS: Vibrational Spectroscopy and Chemical Imaging on the Nanometer Scale" Chair: **Prof. Volker Deckert** *(Friedrich-Schiller University, Germany)*
18:30-20:30	**WELCOME RECEPTION**

24 August 2026, Monday

08:30–-	Registration (open all day)
	HALL 1 - AMPHITHEATER
09:00–09:45	**Plenary: Prof. Katsumasa Fujita** *(The University of Osaka, Japan)* "Engineering Sensitivity and Selectivity in Raman Cellular Imaging: Advanced Illumination and Cryogenic Strategies" Chair: **Prof. Siva Umapathy** *(Indian Institute of Science, India)*
09:45–10:05	**Coffee Break**

Scientific Programme

24 August 2026, Monday

	HALL 1 - AMPHITHEATER (SERS/TERS) Chair: Bin Ren	HALL 2 (NL/TR) Chair: Janina Kneipp	HALL 3 (Coherent-Imaging) Chair: Sumeet Mahajan	HALL 4 (Novel) Chair: Young Mee Jung	HALL 5 (Bio) Chair: Harumi Sato	HALL 6 (Bio/SERS/Pharma) Chair: Antonio Gomes Souza Filho
10:05-10:35	**Keynote: Ado Jorio** *(UFMG, Brazil)*, "Towards quantitative analysis of defects in Tip-Enhanced Raman Spectroscopy of Graphene and other 2D systems"	**Keynote: Tullio Scopigno** *(Universitá di Roma, Italy)*, "Vibrational Dynamics à la Carte: Background-Free Mode-Selectivity by Phase-Controlled Impulsive Raman Spectroscopy"	**Invited: Sandro Heuke** *(Institut Fresnel, CNRS, France)* "4-pulse, 2-color stimulated Raman histology"	**Invited: Jianan Huang** *(University Of Oulu, Finland)* "AI-assisted plasmonic nanopores for single-molecule SERS detection of post-translational modifications"	**Keynote: Jurgen Popp** *(Leibniz Instiute Of Photonic Technology, Germany)* "From Raman Fingerprints to Patients: AI-Driven Translational Raman Spectroscopy for Precision Medicine"	**Keynote: Jaebum Choo** *(Chung Ang University, South Korea)*, "Rapid and Sensitive Pathogen Screening Using SERS Sensors"
10:35-10:55 10:50-10:55	**Invited: Naresh Kumar** *(ETH Zurich, Switzerland)*, "Unravelling Catalytic Reaction Mechanisms with In Situ Tip-Enhanced Raman Spectroscopy"	**Invited: Dongho Kim** *(Yonsei University, South Korea)*, "Structural Evolutions in the Multiexciton Generation Processes in Slip-Stacked Perylene Dye Array probed by Time-resolved Electronic and Vibrational Spectroscopy"	**#22, Florian Matthias Schweizer** *(Max Planck Institute for Solid State Research, Germany)* , Doppler dual-comb coherent Raman spectromicroscopy and holography	**Invited: Vikas Kumar** *(University of Duisburg-Essen, Germany)* "Rapid Coherent-Raman Optical Activity (CARS-ROA) spectroscopy in the low millisecond regime"	**Invited: Takakazu Nakabayashi** *(Ohoku University, Japan)* "Application of Raman Imaging to Liquid-Liquid Phase Separation of Proteins: Quantitative Analysis of Coexisting Components"	**Invited: Lawrence Ziegler** *(Boston University, USA)* "Ultra-rapid, Quantitative, Label-free Antibiotic Susceptibility Testing (AST) via SERS Detected Purine Metabolites: The World's Fastest AST Methodology"
10:55-11:10	**#359, Alice Fiocco** *(HORIBA France SAS, France)*, TERS for analysing lithium-transfer kinetics on cathode active surfaces	**#333, Anna Maria Nowakowska** *(Jagiellonian University, Poland)*, From Molecular Vibrations to Cellular Dynamics: Real-Time Raman Study of Fatty Acid Uptake	**#57, Itsuki Yamamoto** *(The University of Osaka, Japan)*, Time-Lapse 3D SRS Imaging of Multicellular Systems With Reduced Photodamage Using Chirped Picosecond Pulses	**#112, Jana Thissen** *(Institut für Umwelt & Energie, Technik & Analytik e.V. (IUTA), Germany)*, Online Coupling of Size Exclusion Chromatography to Capillary Enhanced Raman Spectroscopy for Biopharmaceutical and Biological Applications	**#310, Aleksandra Pragnąca** *(Jagiellonian University, Poland)*, Spectral signature of hypoxia. Time-dependent effects on brain endothelium revealed by FTIR and Raman imaging	**#466, Deniz Yilmaz** *(Yeditepe University, Turkiye)*, Label-Free Monitoring of Intracellular Pathways via Surface-Enhanced Raman Scattering
11:10-11:25	**#64, Anushree Dutta** *(ETH Zurich, Switzerland)*, Nanoplastics Detection in Complex Cellular Environments by Tip-Enhanced Raman Spectroscopy	**#335, Antti Penttinen** *(Picophotonics Oy, Finland)*, Compact, single-frequency high repetition rate picosecond laser for time-resolved Raman spectroscopy	**#37, Jin Guo** *(Peking University, China)*, A Self-Calibrated High-Speed Delay Scanning System for Time-Domain Stimulated Raman Spectroscopy	**#17, Jessica Gabb** *(IS-Instruments Ltd., United Kingdom)*, A New Raman Spectroscopic Approach to Gaseous Tritium Analysis in the Fusion Fuel Cycle Using Hollow-Core Microstructured Optical Fibres	**#467, Ana Batista de Carvalho** *(University of Coimbra, Portugal)*, Beyond Histology: Detecting Endometrial Polyps through Raman Spectroscopy	**#430, Nihal Simsek Ozek** *(Atatürk University, Turkiye)*, Unlocking the Wound-Healing Potential of {Tarantula cubensis} Venom: Migration, Cytotoxicity, and Raman Spectroscopic Profiling in a Human Dermal Fibroblast Model
11:25-11:40	**#102,Balaji Sanap** *(Tokushima University, Japan)*, Force-Induced Isomerization of azobenzene monitored by Tip-Enhanced Raman Spectroscopy	**#203, Borui Zhang** *(Institut Fresnel, France)*, Impulsive stimulated Raman scattering with multiple pump pulses	**#131, Lilian Magermans** *(Institut Fresnel, France)*, Wide-field Hyperspectral Coherent Anti-Stokes Raman Scattering (CARS) Microscopy using Speckled Illumination	**#77, Keishi Yang** *(The University of Osaka, Japan)*, High-speed AFM/micro-Raman Multimodal Measurement System: Correlative Analysis of Conformational and Chemical-bond Dynamics	**#236, Ion Nesterovschi** *(Babeş-Bolyai University, Romania)*, Raman characterization of blue microplastic ingestion and carotenoid responses in zooplankton	**#74, Giulia Bruno** *(Italian Institute of Technology, Italy)*, Label-Free Evaluation of Drug Effects in Brain Organoids and Spheroids Using Raman Spectroscopy
11:40-11:55	**#204, Dai Zhang** *(Eberhard Karls University of Tübingen, Germany)*, Enhanced Raman spectroscopy for chemical reactions at air-metal interfaces	**#398, Gaia De Maria** *(Sapienza University of Rome, Italy)*, Broadband Stimulated Raman Scattering On Methylene Blue: Probing Equilibrium And Excited State Properties	**#92, Eric Michele Fantuzzi** *(Cambridge Raman Imaging Srl, Italy)*, Single-Shot Multiplex SRS for Rapid Chemical Imaging: Microplastics, FFPE Virtual Histology, and Broader QC Applications		**#601, Deniz Yılmaz** *(Yeditepe University, Turkiye)*, Navigating Complex Biological Platforms: From Nanobiosensors to Bioimaging	
12:00-13:30	**LUNCH**					
	HALL 1 - AMPHITHEATER					
13:30–14:15	**Plenary: Prof. Siva Umapathy** *(Indian Institute Of Science, India)* "Impact of Artificial Intelligence in Raman Spectroscopy in Basic Research and Societal Applications" Chair: **Prof. Tullio Scopigno**					

Scientific Programme

24 August 2026, Monday

14:15–14:35	Coffee Break					
	HALL 1 - AMPHITHEATER (SERS/TERS) Chair: Jianan Huang	**HALL 2 (NL/TR) Chair: Dongho Kim**	**HALL 3 (Coherent-Imaging) Chair: Haluska Miroslav**	**HALL 4 (Novel) Chair: Vikas Kumar**	**HALL 5 (Bio) Chair: Kamilla Małek**	**HALL 6 (SERS/TERS) Chair: Kumar Naresh**
14:35-14:55	**Invited: Sangwoon Yoon** *(Chung-Ang University, South Korea)*, "Plasmonic Photothermal Phase Transition of TiO2 Nanoshells around Gold Nanorods"	**Invited: Hideaki Kano** *(Keio University, Japan)*, "Label-Free Detection of Cardiac Amyloid Deposits in Human Tissue by Multiplex CARS Spectroscopic Imaging",	**Invited: Hanqing Xion** *(Peking University, China)*, "Super-broadband stimulated Raman scattering spectroscopy and imaging"	**Invited: Hyung Min Kim** *(Kookmin University, Korea)*, "Development of Macro- and Microscale Line-scan Raman Systems for Environmental Monitoring"	**Invited: Samir F. El-Mashtoly** *(Leibniz Institute of Photonic Technology, Germany)*, "Bioorthogonal Vibrational Probes Enable Raman Imaging of Enzyme Activity in Cells"	**Invited: Rostislav Bukasov** *(Nazarbayev University, Kazakhstan)* "Looking beyond gold and silver, quest for inexpensive but efficient SERS substrates in sandwich immunoassays with SERS readout and SERS for detection of proteinuria"
14:55-15:10	**#207, Felix Schneider** *(University of Tübingen, Germany)*, Angular Distribution of Tip-Enhanced Raman Scattering	**#356, Giovanni Batignani** *(Sapienza University of Rome, Italy)*, Temperature Dependence of Stimulated Resonant Raman Scattering	**#373, Luca Genchi** *(Institut Fresnel, France)*, CARS endoscopy through an ultra-thin multi-core fiber	**#472, Montserrat Roman Quintero**,*(Humboldt-Universität zu Berlin, Germany)*, Interfacial Vibrational Spectroscopic Insights into Membrane Disruption using Antimicrobial Peptides	**#13, István Csarnovics,** *(University of Debrecen, Hungary)*, LabelFree Raman Spectroscopy for Discriminating Breast Cancer Cell Lines and Macrophage Polarization States	**#457, Melike Sarıçam**, *(TÜBİTAK MAM, Turkiye)*, From Lab to Field: Enhancing SERS Detection of Dipicolinic Acid through Sampling-Relevant Chemical Activation Using Commercial Substrates and a Portable Raman Spectrometer
15:10-15:25	**#206, Gleb Tselikov** *(XPANCEO, United Arab Emirates)*, Hyperbolic-enhanced Raman spectroscopy of 2D materials on natural vdW $MoOCl_2$	**#363, Karolina Skała** *(Institute of Physical Chemistry, Polish Academy of Sciences, Poland)*, Vibrational enhancement in $Au_{25}(PET)_{18}$ nanoclusters probed by Stimulated Raman Spectroscopy	**#384, Marco Da Ros** *(Politecnico di Milano, Italy)*, Multimodal Nonlinear Raman Imaging For Label-Free Histology Of Head And Neck Tumor Microarrays	**#341, Morteza Behrouzitabar** *(University of Milano-Bicocca, Italy)*, Full Vibrational Spectroscopy for Simultaneous Mechanical, Structural and Chemical Analysis	**#465, Jorge Perez-Juste** *(Universidade de Vigo, Spain)*, Light-Responsive Plasmonic Nanoparticle-Bacterial Biohybrids for Targeted and Multiplexed SERS Imaging	**#39, Shathar Alobeidat** *(University of Trieste, Italy)*, Validated Quantitative SERS Method for Trace Pharmaceutical Detection
15:25-15:40	**#211, Ario Jafari** *(Linköping University, Sweden)*, Quantitative SERS of PEDOT:PSS using nanocellulose–Au@Ag nanowire composite films	**#306, Koichi Iwata** *(Gakushuin University, Japan)*, Initial Phase of Bimolecular Reactions between {p}-Terphenyl Derivatives and Carbon Tetrachloride Detected by Picosecond Time-resolved Raman Spectroscopy	**#512, Max Brinkmann** *(Refined Laser Systems GmbH, Germany)*, (Refined Laser Systems GmbH, Germany), Feature level validation of label-free intraoperative histology in glioblastoma using stimulated raman scattering imaging	**#293, Andrii Kutsyk** *(Lightnovo ApS, Denmark)*, qRICO-Net: machine-learning-based crystallographic orientation mapping using polarized Raman microscopy	**#36, Joseph O'Halloran** *(Foshan University, China)*, (Tyndall National Institute, Ireland), Monte Carlo Based Quantitative Spatially Offset Raman Spectroscopy Towards Non-Invasive Bone Quality Assessment	**#328, Shilong Zhao** *(Foshan University, China)*, Moiré tunable Raman enhancement in twisted MnPS3
15:40-15:55	**#461, Arna Ghosh**, *(Leibniz Institute of Photonic Technology, Germany)*, Detection To Degradation: A SERS Strategy for Tackling Benzotriazole in Complex Water Matrices	**#357, Marcin Pastorczak**, *(Institute of Physical Chemistry, Polish Academy of Sciences, Poland)*, The Origin of the Frequency-Dependence of the OH Stretch Vibrational Lifetimes in Liquid Water – Polarization-Resolved fs-IR Pump – Stimulated Raman Probe Study	**#210, Ruidong Ji**, *(University of Bath, United Kingdom)*, Hybrid CW–Pulsed Coherent Anti-Stokes Raman Scattering	**#342, Anna Lisa Gilioli**, *(University of Turin, Italy)*, Identification and quantification of nanoplastics using Raman spectroscopy optimised by dielectrophoretic pre-concentration	**#152, Karolina M. Turczyńska***(Jagiellonian University, Poland)*, Raman spectroscopic analysis of nanoparticle uptake dynamics in human cells	**#28, Shrobona Banerjee***(Humboldt-Universität zu Berlin, Germany)*, Protein-gold nanoparticle interface characterized by machine learning-assisted surface enhanced Raman scattering (SERS)
15:55-16:10	**#242, Barbara Palys**, *(University of Warsaw, Poland)*, Conducting Polymer-Functionalized Gold Nanoparticles As A Reactive Oxygen Species SERS Reporters	**#284, Masanari Okuno**, *(The University of Tokyo, Japan)*, Polarization-resolved spontaneous nonlinear scattering captures phonon-like motion in liquids	**#49, Shun Takahashi** *(The University of Tokyo, Japan)*, Stimulated Raman Scattering Imaging of Dislocation-Induced Strain Fields in Bulk GaN Substrates,	**#8, Bogdan Sava***(attocube systems GmbH, Germany)*, Multimodal Nanoscale Materials Characterization via Correlative Nano-IR, Raman Microscopy, and Atomic Force Microscopy	**#73, Lucía Ronda** *(Lightnovo ApS, Denmark)*, Raman Spectroscopy for Bacterial Identification: From Full Cultivation to In Vivo Measurements	**#441, Sinan Genc***(Abdullah Gül University, Turkiye)*, Low-Cost, Scalable SERS Substrates Based on Copper-Assisted Chemically Etched Silicon with Inverted Surface Architectures
16:10-19:00	**POSTER SESSION AND MIXER**					

Scientific Programme

25 August 2026, Tuesday

	HALL 1 - AMPHITHEATER					
09:00–09:45	**Plenary: Prof. Isabel Pastoriza-Santo** *(Universidade De Vigo, Spain)* "Engineering Plasmonic Nanostructures For Next-Generation SERS-Based Detection" Chair: **Prof. Emiliano Cortés** *(University of Munich, Germany)*					
09:45–10:05	**Coffee Break**					
	HALL 1 - AMPHITHEATER (SERS/TERS) Chair: Volker Deckert	**HALL 2 (NL/TR) Chair: Ozaki Yukihiro**	**HALL 3 (Coherent-Imaging) Chair: Mustafa Kansiz**	**HALL 4 (Novel) Chair: Ado Jorio**	**HALL 5 (Bio) Chair: Jaebum Choo**	**HALL 6 (NL/TR) Chair: Thomas Bocklitz**
10:05-10:25	**Keynote:** **Bin Ren** *(Xiamen University, China)* "Electrochemical Tip-enhanced Raman Spectroscopy--More than 10 years development, current status and future opportunity'	**Keynote:** **Simion Astilean** *(Babes Bolyai University, Romania)* "Multifunctional Plasmonic Nanoplatforms for SERS, Bioimaging and Plasmon-Enhanced Therapies"	**Keynote:** **Ji-Xin Cheng** *(Boston University, USA)* "Stimulated Raman Photothermal Microscopy: Chemical imaging with high sensitivity and ease of operation"	**Keynote:** **Sumeet Mahajan** *(University of Southampton, UK)* 'Multi-Excitation Raman Spectroscopy and its Applications in Biology and Medicine'	**Invited:** **Yasuyuki Ozeki** *(The University of Tokyo, Japan)* Stimulated Raman Scattering Microscopy For Cellular Analysis And Semiconductor Characterization	**Keynote:** **Thomas Bocklitz** *(Friedrich Schiller University, Germany)* "Extending the photonic data science toolbox: Data Infrastructure Methods and Physically Inspired Deep Learning Models'
10:05-10:35						
10:35-10:55	**Invited:** **Rares Stiufiuc** *(Regional Institute Of Oncology Iasi, Romania)* "SERS-Based Analysis of Biological Fluids for Liquid Biopsy Applications"		**#499, Shupeng Zhao** *(Laboratoire Kastler Brossel, France)*, Chemical imaging through scattering medium	**Invited:** **Torsten Frosch** *(TU Darmstadt, Germany)* Advanced Drug Monitoring of Anti-infectives Exploiting Deep-UV Raman Spectroscopy and Fiber Sensors	**Invited:** **Peter Mojzeš** *(Charles University, Czech Republic)* "Characterization of Molecular Crystals Produced by Microalgae by Means of Raman Microscopy"	**Invited:** **Ion Notingher/Radu Boitor** *(University of Nottingham, UK)* "Raman spectroscopy techniques for intra-operative diagnosis in cancer surgery"
10:50-10:55						
10:55-11:10	**#219, Cecilia Spedalieri** *(Humboldt-Universität zu Berlin, Germany)*, Probing intracellular interactions of functionalized nanoparticles for organelle targeting with SERS	**#315, Miroslav Kloz** *(ELI Beamlines Facility, Czech Republic)*, Vibrational signature of 1Bu+ and hot 2Ag- excited states of carotenoids revisited by femtosecond stimulated Raman spectroscopy	**#9, Yang Ma** *(The University of Tokyo, Japan)*, Fast and Low-Power Super-Resolution Vibrational Imaging Enabled by an Improved Photoswitchable Raman Probe	**#479, Chengxiang Jin** *(Institute for Molecular Science, Japan)*, Coherent Raman spectroscopy for buried interfaces via spatiotemporal field engineering	**#395, Gergo Peter Szekeres** *(Freie Universität Berlin, Germany)*, Vibrational probing of the glycosaminoglycan structure-function relationship through physicochemical perturbation	**Invited:** **Nina Jeliazkova** *(Ideaconsult Ltd, Bulgaria)* "FAIR Analytical Data for Safe and Sustainable by Design"
10:55-11:15						
11:10-11:25	**#303, Dana Cialla-May** *(Leibniz Institute of Photonic Technology, Germany)*, SERS-Based Drug Monitoring and Biomarker Detection in Complex Biological Matrices	**#414, Neethish Madathiparambil Mohanan** *(Sapienza University of Rome, Italy)*, Harnessing the coupling of photocarriers to lattice displacements in low dimensional perovskites: an impulsive vibrational spectroscopy perspective	**498, Yaren Sarıboğa** *(Ozyegin University, Turkiye)*, Burst-Mode femtosecond lasers for enhanced stimulated raman spectroscopy	**#71, Felix Schröter** *(Federal Institute for Materials Research and Testing (BAM), Germany)*, Rapid Microplastic Imaging enabled by a pulsed UV Raman Microscope	**#238, Martyna Anna Pytlarz** *(Technical University of Denmark, Denmark)*, Discrimination And Quantification Of Methotrexate In The Presence Of Its Metabolites And Co-administrated Drugs In Patient Serum Using Lab-On-Disc SERS Platform Supported By Multivariate Data Analysis	**#0321, Jamile Jafari** *(Leibniz Institute of Photonic Technology, Germany)*, Towards FAIR Raman and IR Spectroscopy: A Minimal Metadata Framework
11:25-11:40	**#290, David Baschnagel** *(Eberhard Karls University Tübingen, Germany)*, Angularly Resolved Raman Spectroscopy of Cobalt(II)phtalocyanine through a Particle on Mirror System	**#470, Roozbeh Bonakdar** *(Özyeğin University, Turkiye)*, Accelerating raman spectroscopy imaging via fine-tuned diffusion models for sparse data reconstruction	**#279, Yusuke Murakami** *(Kyushu University, Japan)*, Broadband electronic resonance coherent anti-Stokes/Stokes Raman scattering microscopy for High-Speed and High-Sensitivity Imaging of Biomolecules	**#431, Hankun Yang** *(Laboratoire Kastler Brossel, France)*, Asynchronous Ultrafast Spontaneous Raman Sensing	**#331, Maryam Jebari Ben Omar** (*CIC nanoGUNE, Spain)*, Label Free Assessment Of Spermatozoa Status	**#129, Shuxia Guo** *(Leibniz Institute of Photonic Technology, Germany)*, Machine learning and data science in IR spectroscopy for biomedical applications
11:40-11:55	**#286, Eungyeong Park** *(Kangwon National University, South Korea)*, SERS-based detection of cancer cell surface proteins for early cancer diagnosis	**#501, Ryu Yoshizawa** *(Institute for Molecular Science, Japan)*, Probing microscopic network structure in ultrathin amorphous layers by time-frequency hybrid coherent Raman spectroscopy	**#437, Samuel Brito Ferreira Santos** *(University of Strathclyde, UK)*, Monitoring pharmaceutical isolation processes through Spatially Offset Raman Spectroscopy: dilution- and displacement-driven filtration-washing	**#389, Nicolai Jonathan E. Jacobsen** *(Lightnovo ApS, Denmark)*, Miniature Raman Spectrometer with Tunable Laser for Minerals Research	**#136, Muhammad Asyraf Onn** *(Technological University Dublin, Ireland)*, Multimodal Raman and Infrared O-PTIR Spectroscopy for Detection of Transforming hr-HPV Infection in Single Cervical Cells	**#0199, Andrei Markin** *(Renishaw PLC, United Kingdom)*, Suppressing spectral backgrounds with time-resolved Raman spectroscopy (TRRS)
12:00-13:30	**LUNCH/ICORS Steering Committe Meeting**					

Scientific Programme

25 August 2026, Tuesday

	HALL 1 - AMPHITHEATER					
13:30–14:15	**Plenary: Ramón A. Alvarez-Puebla** *(Universitat Rovira i Virgili, Spain)*, "Plasmonic porous materials and their applications in SERS" Chair: **Zenobi Renato** *(ETH Zurich, Switzerland)*					
14:15–14:35	**Coffee Break**					
	HALL 1 - AMPHITHEATER (SERS/TERS) Chair: Dae Hong Jeong	**HALL 2 (NL/TR) Chair: Paul Champion**	**HALL 3 (Materials) Chair: Hyeonsik Cheong**	**HALL 4 (Novel) Chair: Liqing Zheng**	**HALL 5 (Bio) Chair: Hugh Byrne**	**HALL 6 (Bio) Chair: Samir Elmastholy**
14:35-14:55	**Invited: Sebastian Schlücker** *(University of Duisburg Essen, Germany)* "Probing a reactive alkyne centre aligned by a rigid molecular tripod by single-molecule TERS for electric field-induced chemistry'	**Invited: Harumi Sato** *(Kobe University, Japan)* "Visualization of In-Situ Marine Biodegradation in Poly(3-hydroxybutyrate) Using Three-Dimensional Raman Mapping"	**Invited: Hyeonsik Cheong** *(Sogang University, South Korea)* "Raman spectroscopy for magnetic two-dimensional materials"	**Invited: Katarzyna Majzner** *(Jagiellonian University, Poland)* "Decoding drug response across systems: Raman insights from endothelium to leukemia"	**Invited: Kamilla Malek** *(Jagiellonian University, Poland)* "Raman and FTIR Imaging Sensitivity and Specificity in Decoding Cellular Transformations and Dysfunctions in 2D and 3D In Vitro Models"	**Invited: Agnieszka Kamińska** *(Polish Academy of Sciences, Poland)* "Biomedical and analytical applications of SERS supported by machine learning: Towards development of the novel tool for clinical diagnosis"
14:55-15:10	**#193, Eva Kočišová** *(Charles University, Czech Republic)*, Photocatalytically Recyclable Nb_2O_5/Metal Hybrid Platforms For Surface-Enhanced Raman Scattering (SERS) Spectroscopy	**#41, Jitendra Acharyya** *(Institut Fresnel, France)*, Intrinsic backward emission of coherent Raman photons from homogeneous media	**Invited: Simona Cintă Pinzaru** *(Babes Bolyai University, Romania)* "Aquatic Aged Micro-Nano Plastic Reference Materials as Resonance Raman-SERRS Traceable Probe for Controlled Exposure and Impact Studies"	**#345, Polina Kasyanova** *(Max Planck Institute for the Science of Light, Germany)*, Toward Single-Particle Raman Microscopy of Vitrified Biological Samples at Liquid Helium Temperature	**#408, Parvin Ghalebtarash** *(Leiden University, Netherlands)*, High-Throughput Compressed-Sensing Raman Microscopy for Label-Free Cellular Differentiation Analysis	**#091, Danylo Komisar** *(Lightnovo ApS, Denmark)*, DTNR-SORS: A Hardware Solution to the Sensitivity Bottleneck in Raman Glucose Sensing
14:55-15:15						
15:10-15:25	**#60, Giulia Spaggiari** *(CNR-IMEM, Italy)*, A Multi-scanning-probe Study of Local nanoscale Properties in Cu-Doped Sb_2Se_3 Photovoltaic Films	**#311, Sergey G Pavlov** *(German Aerospace Center (DLR), Germany)*, Lattice dynamics of transparent rock-forming minerals probed by complementary frequency-domain and time-domain Raman spectroscopy	**#334, Alicia Gómez López** *(Instituto de Catálisis y Petroleoquímica, CSIC, Spain)*, Comparing Smoothing Methods for Noise Reduction in Raman Spectroscopy: Impact on Plastics Identification	**#321, Václav Profant** *(Charles University, Czech Republic)*, Terahertz Raman Optical Activity as a Window into G-Quadruplex Self-Assembly	**#253, Patrycja Dawiec** *(Jagiellonian University, Poland)*, Raman Spectroscopic Analysis of Fatty Acid Synthase and Cholesterol Inhibition in Blood Cancers	**#065, Ewa Pięta** *(Institute of Nuclear Physics Polish Academy of Sciences, Poland)*, Multimodal spectroscopic evidence of selective cytotoxic and radiosensitizing effects of withaferin A in cervical cancer cells
15:25-15:40	**#241, Gohar Soufi** *(Technical University of Denmark, Denmark)*, Automated Sample Pretreatment of Complex Matrices on a Centrifugal Microfluidic Platform for Nanopillar-Assisted Separation and SERS Detection	**#427, Jacopo Zini** *(University of Helsinki, Finland)*, Alternative Application of Time-Gated Raman Spectrometer: Leveraging Picosecond Time-Gating for Fluorescence Lifetime Sensing of Molecular Diffusion in Collagen Hydrogels	**#121, Dmitry Smirnov** *(National High Magnetic Field Laboratory, USA)*, High-field magneto-Raman spectroscopy of quantum magnets	**#103, Ventsislav K. Valev** *(University of Bath, United Kingdom)*, Meta-Raman Optical Activity	**#125, Sreeparna Nath** *(ACTREC-TMC, India)*, Raman Spectroscopy for Detection of Tyrosine Kinase Inhibitor Resistance in Chronic Myelogenous Leukemia	**#380, Karolina Chrabąszcz** *(Institute of Nuclear Physics Polish Academy of Sciences, Poland)*, From Cells to Isolated Lipid Droplets: Raman Spectrolipidomics of Treatment Response
15:40-15:55	**#220, Hyejin Chang** *(Kangwon National University, South Korea)*, Dual-Enhanced SERS Platforms Using Edge-Engineered Graphene Quantum Dots and Silver Nanoshells	**#322, Shilpa Kurupath Bhavadas** *(ELI ERIC, Czech Republic)*, Mapping the Vibrational States in Retinal and Retinal Schiff Base by FSRS	**#397, Emanuele Mai** *(Sapienza University of Rome, Italy)*, Ultrastability and Hyperageing in Amorphous Materials: Polarization Resolved Stimulated Raman Spectroscopy of Fossil Amber	**#287, Vít Pavelka** *(Institute of Analytical Chemistry of the Czech Academy of Sciences, Czech Republic)*, Plasmonic Microspheres in Flow: Acoustofluidic Focusing for Sensitive SERS Detection	**#85, Timea Frosch** *(Leibniz-Institute of Photonic Technology, Germany)*, Stage-Dependent Mechanisms of Action of Antimalarial Drugs on Hemozoin Formation in Infected Erythrocytes	**#485, Katarzyna Pogoda** *(Institute of Nuclear Physics PAN, Poland)*, Multimodal Raman and AFM-IR nanospectroscopy of plasma membrane vesicles reveals cell-origin dependent membrane composition
15:55-16:10	**#500, Ilayda Alparslan** *(Middle East Technical University, Turkiye)*, Direct Laser Written Periodic Nanostructures for Surface-Enhanced Raman Spectroscopy	**#135, Yoonsoo Pang** *(Gwangju Institute of Science and Technology, South Korea)*, Ultrafast charge transfer dynamics probe by time-resolved Raman spectroscopy	**#198, Jennifer Ferguson** *(Renishaw PLC, United Kingdom)*, Understanding The Impact Of The Fabrication Process On Li-ion Battery Anodes Using Chemical Analysis With The Strada® Intelligent Raman Microscope	**#87, Yaroslav Aulin** *(Lightnovo ApS, Denmark)*, Gemstones and Minerals Identification Using Machine Learning Assisted Raman Spectroscopy	**#524, Mustafa Kansiz** *(Photothermal Spectroscopy Corp, USA)*, Multimodal High-Speed Laser-Scanning Submicron Infrared (O-PTIR) and Stimulated Raman (PT-SRS) Platform for Real-Time Label-Free Chemical Imaging	**#130, Vasundhara Tyagi** *(National Physical Laboratory, United Kingdom)*, Optimisation of through-vial Raman analysis of turbid samples by modelling the Raman intensity-depth decay response
16:10-19:00	**POSTER SESSION AND MIXER**					

Scientific Programme

26 August 2026, Wednesday

	HALL 1 - AMPHITHEATER					
09:00–09:45	**Plenary: Emiliano Cortés** *(University of Munich, Germany)*, "Raman Spectroscopy for Energy Interfaces and Catalysis" Chair: **Katsumasa Fujita** *(The University of Osaka, Japan)*					
09:45–10:00	Announcement of Poster Awards					
10:00–10:15	**Coffee Break**					
	HALL 1 - AMPHITHEATER (SERS/TERS) Chair: Mine Altunbek	**HALL 2 (TC/Geo/Material) Chair: Guillermo Lopez**	**HALL 3 (Imaging/SERS/TERS) Chair: Ugur Tamer**	**HALL 4 (Materials/Pharma) Chair: Duohai Pan**	**HALL 5 (Bio) Chair: Ismail H. Boyaci**	**HALL 6 (NL/Env/Bio) Chair: Elif Öztürk**
10:15-10:35	**Keynote: Janina Kneipp** *(Humboldt Universität Zu Berlin, Germany)* "Biochemistry of lipid metabolism of animal cells as probed by surface-enhanced Raman scattering"	**Invited: Tommaso Giovannini** *(University of Rome Tor Vergata, Italy)* "From Nanoplasmonics to Surface-Enhanced Spectroscopies: an Atomistic Perspective"	**Keynote: Young Mee Jung** *(Kangwon National University, South Korea)* "Versatility and Applications of Raman Spectroscopy in Bioassays"	**Keynote: Antonio Gomes Souza Filho** *(Univesidade Federal Do Ceará, Brazil)* "2D maerials under high-pressure conditions: strain effects on the phonon spectrum"	**Keynote: Hugh J. Byrne** *(Technological University Dublin, Ireland)* "Raman microscopic analysis of cellular function in vitro"	**Invited: Ingo Rimke** *(Ape Gmbh, Germany)* "Highly sensitive and fast hyperspectral SRS image acquisition as well as TPE microscopy with shot noise limited OPO-based light source"
10:35-10:45						
10:45-11:00	**Invited: Omer Aydin** *(Erciyes University, Turkiye)* "AI-Assisted Surface-Enhanced Raman Spectroscopy from Spectral Fingerprints to Diagnosis"	**#139, Giacomo D'Arcangelo** *(Scuola Normale Superiore, Italy)*, Why Do Raman Features Change with Excitation Wavelength? How Resonance States Shape Raman Spectra	**#423, Markéta Benešova** *(Institute of Scientific Instruments of the CAS, Czech Republic)*, Time-lapse metabolic fingerprinting of bacterial stress responses using surface-enhanced Raman spectroscopy	**Invited: Jose Antonio Manrique** *(Universidad De Valladolid, Spain)* "Diverse mineralogies characterized with SuperCam Raman and luminescence in Jezero Crater"	**Invited: Murali Krishna Chilakapati** *(Tmc Actrec, India)* "Minimally Invasive Raman Spectroscopy: Applications for Oral Cancer Assessment"	**#340, Aradhana Dwivedi** *(Leibniz Institute of Photonic Technology, Germany)*, Towards SERS-Based Sensing Platforms for Therapeutic Drug Monitoring in Complex Biofluids
10:45-11:05						
11:05-11:20	**#134, Ahmed Y. F. Mahmoud** *(Technological University Dublin, Ireland)*, In-solution SERS for Liquid Biopsies using a Portable Raman Device for Point-of-care Testing	**#495, Gianluca Serra** *(Politecnico di Milano, Italy)*, Nanographenes' shapes: effects of molecular geometry on Raman spectra from density functional theory	**#348, Mateusz Kasztelan** *(Wageningen University & Research, Netherlands)*, Self-Assembled Core-Shell Nanoparticles For SERS Detection Of Fungal Secondary Metabolites	**#237, Kseniia Makarova** *(Saint Petersburg State University, Russia)*, Gold nanoparticle-catalyzed oxidation of beta-blockers: SERS and capillary electrophoresis study	**#374, Victor Alcolea-Rodriguez** *(CNR-IFN, Italy)*, Label-Free Raman Spectroscopy in Head and Neck Squamous Cell Carcinoma: From Tumor Biopsies to Therapy Response Monitoring in Patient-Derived Tumor Slice Cultures	**#382, Carolin Borbeck** *(Photothermal Spectroscopy Corp GmbH, Germany)*, Smaller Plastics, Bigger Risks: Correlative Raman and O-PTIR Microspectroscopy for High-Confidence Identification of Submicron Microplastics
11:20-11:35	**#30, Ana Luiza Clivatti Yamanaka** *(Universidade de São Paulo, Brazil)*, Controlling Gold Nanoparticles Electrodeposition for Reproducible SERS Substrates on Transparent Electrodes	**#43, Jesper Sand** *(Technical University of Denmark, Denmark)*, Evaluating And Choosing Experimental Parameters For Shifted Excitation Raman Difference Spectroscopy: A Quantitative Study	**#489, Serpil Harbeck** *(TÜBİTAK MAM, Turkiye)*, Detection of Chemical Warfare Agent Simulants on Commercial Substrates via Surface-Enhanced Raman Spectroscopy	**#402, Krystian Pupel** *(University of Warsaw, Poland)*, Tracking Structural Changes in Graphene Oxide: From Established Raman Signatures to Fragmentation Effects	**#90, Zeynep Kilinc** *(University of Health Sciences, Turkiye)*, Systematic Investigation of Drug Resistance Reversal in Triple Negative Breast Cancer Using Raman Spectroscopy	**#227, Siddarth Shivkumar** *(National Physical Laboratory, United Kingdom)*, Metrology For Coherent Raman Scattering Microscopy
11:35-11:50	**#120, Ana Luiza Correa Januário** *(Universidade de São Paulo, Brazil)*, Modulating SERS and Enhanced Fluorescence of Copper Complexes Through Silica Shell Thickness in Ag@SiO_2 Nanoparticles	**#151, Marc Bröckel** *(Eberhard Karls Universität Tübingen, Germany)*, Atomic Contributions to the Raman Intensity Reveal Molecular Charge Density Shifts – a combined Experimental and Computational Approach	**#447, Munevver Akdeniz** *(Erciyes University, Turkiye)*, SERS-Based Label-Free Exosome Profiling for Acute Leukemia Detection via Machine Learning	**#302, Luis Gómez Fernández** *(University of Cantabria, Spain)*, Water-vapor induced crystal transformation from the Jahn-Teller Rb2CuCl4 to the Pseudo Jahn-Teller Rb2CuCl4(H2O)2: Diffusion dynamics study		**#67, Paul Finnie** *(National Research Council Canada, Canada)*, The structure of Raman excitation maps from pure carbon nanotube materials

Scientific Programme

26 August 2026, Wednesday

	HALL 1 - AMPHITHEATER (SERS/TERS) Chair: Mine Altunbek	HALL 2 (TC/Geo/Material) Chair: Guillermo Lopez	HALL 3 (Imaging/SERS/TERS) Chair: Ugur Tamer	HALL 4 (Materials/Pharma) Chair: Duohai Pan	HALL 5 (Bio) Chair: Ismail H. Boyaci	HALL 6 (NL/Env/Bio) Chair: Elif Öztürk
11:50-12:05	**#332, Angelika Łepek** *(Gdańsk University of Technology, Poland)*, Rapid manufacturing of nanostructured carbon-based EC-SERS platforms functionalized with gold nanoparticles	**#94, Iona Elizabeth Hill** *(Edinburgh Instruments, United Kingdom)*, Polarised Raman and Second Harmonic Generation Microscopy for Probing Symmetry, Strain, and Layer Interactions in Two Dimensional Materials	**#5, Peilin Xin** *(University of Oulu, Finland)*, Single-Molecule Monitoring of Nucleic Acid Dynamics Using Raman Correlation Spectroscopy in Plasmonic Nanowells	**#409, Miklos Veres** *(HUN-REN Wigner Research Centre for Physics, Hungary)*, Incorporation of nitrogen into nanocrystalline diamond - a multi-wavelength Raman spectroscopic study	**#481, Rami Zewail** *(Egypt-Japan University of Science and Technology, Egypt)*, Continual Learning Strategies for Sequential Pathogen Update in Raman Spectroscopy-Based Identification	**#401, Hemanth Nothalapati** *(Shimane University, Japan)*, From Accuracy to Interpretability: Explainable AI for Reliable Classification of Cancer Cells Using Raman Spectroscopy
12:05-12:20	**#104, Anton Minnekhanov** *(XPANCEO, United Arab Emirates)*, Natural hyperbolic $MoOCl_2$ for anisotropic Raman and SERS-like enhancement	**#202, Miriam Boehmler** *(WITec GmbH, Oxford Instruments, Germany)*, In situ Confocal Raman Spectroscopy and Microscopy from Cryogenic to Extreme High Temperatures: Monitoring Material Behaviour Across Wide Thermal Ranges	**#244, Sampurno Banerjee** *(ACTREC-TMC, India)*, Misclassification-Driven Insights into Abnormal Changes in the Hamster Buccal Pouch: A Serum Raman Spectroscopy Approach	**#390, Ivan Němec** *(Charles University,Czech Republic)*, Study of Polymorphism in the Family of Guanidine-based Molecular Crystals for Nonlinear Optics	**#107, Alessio Sacco** *(Istituto Nazionale di Ricerca Metrologica, Italy)*, Dielectrophoresis enhancement of Raman spectroscopy in liquid for biological characterizations: viruses, bacteria and eco-coronas on nanoplastics	**#320, Priyanka Arun Jadhav** *(Tata Memorial Centre (TMC),India)*, Serum Raman Spectroscopy and Metabolomics Reveal Early Events in Oral Carcinogenesis
19:30-23:00	**Gala Dinner on Boat**					

Scientific Programme

27 August 2026, Thursday

HALL 1 - AMPHITHEATER					
09:00–09:45	**Plenary: Prof. Jian-Feng Li** *(Xiamen University, China)* "In-Situ Raman Probing Surface Reactions" Chair: **Prof. Sebastian Schlücker** *(University of Duisburg Essen, Germany)*				
09:45–10:05	**Coffee Break**				
	HALL 1 - AMPHITHEATER (SERS/TERS) Chair: Yuika Saito	**HALL 2 (Materials) Chair: Jihyeon Yeom**	**HALL 3 (Industrial / Materials) Chair: Ilgin Nar**	**HALL 4 (SERS/TERS) Chair: Karolina Turczyńska**	**HALL 5 (Bio/Theory) Chair: Katarzyna Majzner**
10:05-10:25	**Invited:** **Shuang Guo** *(Jilin Normal University, China)* "Regulation Mechanisms of SERS Activity in Organic Semiconductor Composites"	**Invited:** **Chiara Cappelli,** *(Scuola Normale Superiore, Pisa, Italy)* Atomistic Modeling of Raman Spectra in Complex Environments: From Solutions to Surface-Enhanced Raman Scattering	**Invited:** **Duohai Pan** *(Bristol Myers Squibb, USA)* "Raman Spectroscopy and microscopy for Accelerated Pharmaceutical Development: Applications from Preclinical to Commercialization"	**Keynote:** **Volker Deckert** (*Friedrich-Schiller University, Germany)* "Tips and fields - pushing Raman resolution"	**Invited:** **Matteo Tommasini** *(Politecnico Di Milano, Italy)* "Vibrational spectroscopy under external electric fields: probing molecular structure and interactions"
10:25-10:35					
10:35-10:40	**#344, Anja Boisen** *(Technical University of Denmark, Denmark)*, Active SERS platforms: Light-Driven Micromotors and Living Algae	**#201, Hirotsugu Hiramatsu** *(National Yang Ming Chiao Tung University, Taiwan)*, Sugar analysis in honey using HILIC-Raman technique	**#396, Akif Goktug Bozkurt** *(Ardahan University, Turkiye)*, Discrimination of Regional Honey Samples from Northeastern Türkiye Using Raman Spectroscopy	**Invited:** **Dae Hong Jeong** *(Seoul National University, South Korea)* "Surface-enhanced Raman Optical Activity of Molecules using Chirality Induction from Chiral Molecules to Non-chiral Molecules on a Particle-on-Film Substrate"	**Invited:** **Fiona Lyng** *(Technological University Dublin, Ireland)* "Raman Spectral Cytopathology: A Minimally Invasive Approach for Early Detection of Pre-Cancerous Lesions"
10:40-10:55					
10:55-11:10	**#417, Irving Brian Becerril Castro** *(Universitat Rovira i Virgili, Spain)*, Rapid Inkjet Fabrication of Modular Plasmonic Chemosensors	**#63, Mirosław Mączka** *(Polish Academy of Sciences, Poland)*, Vibrational Studies of Phase Transitions in Multilayered Hybrid Lead Halide Perovskites	**#413, Marco Agozzino** *(Politecnico di Milano, Italy)*, Exploring The Length Saturation Limit Of Carbon Atomic Wires By UV Resonant Raman Spectroscopy	**#34, Yuge Liang** *(University of Oulu, Finland)*, Raman spectroscopic of single-live-cell membrane electrical penetration dynamics via plasmonic nanotubes	**#230, Sungjun Kwak** *(Seoul National University, South Korea)*, Affinity-driven SERS detection of natural dyes using hydrophobic interaction and coordination bonding
11:10-11:25	**#326, Elena Tolstik** *(Leibniz-Institut für Analytische Wissenschaften – ISAS, Germany)*, Multimodal Cardiac Tissue Analysis Using Raman Spectroscopy and AP-MALDI Mass Spectrometry Imaging in a Mouse Model of Lysosomal Storage Disease	**#31, Ruben F. Kranenburg** *(The Netherlands Police / University of Amsterdam, Netherlands)*, Deep-UV Resonance Raman Spectroscopy Enables Reliable MDMA Identification in Colored Ecstasy Tablets	**#147, Ané Kritzinger** *(The University of Adelaide, Australia)*, Fluorescence suppression techniques for through-container Raman spectroscopy	**Invited:** **Liqing Zheng** (Nanjing University, China) "Nanoscale chemical imaging of interfacial reactions by tip-enhanced Raman spectroscopy"	**Invited:** **Roman Holomb** *(Institute for Solid State Physics and Optics Hungary)* "Detection of single nucleotide variants using alkyne-tagged Raman-active DNA probes"
11:25-11:30					
11:30-11:45	**#21, J ingwen Zhou** *(Xiamen University, China)*, Noninvasive Breath-Based Monitoring of Oxidative Stress via Photoinduced Charge-Transfer Mechanisms	**#285, Sabrina Hakelberg** *(Oxford Instruments WITec, Germany)*, Correlative Raman Microscopy Across Disciplines: From Cellular Architecture to 2D Material Heterostructures	**#458, Eda Kiriş** *(Istanbul University-Cerrahpasa, Turkiye)*, Discrimination of Ballpoint Pens and Analysis of Artificially Aged Document with Confocal Raman Spectroscopy	**#75, Wenjun Chen** *(Foshan University, China)*, Two-Dimensional Thiophosphites Enhanced Raman Scattering: From Sub-Zeptomolar Sensing to SixteenOrder-of-Magnitude Quantitative Analysis	**#368, Oleksii Ilchenko** *(Lightnovo ApS, Denmark)*, Deviations from inverse-square law in standoff Raman spectroscopy
11:45-12:00	**#508, Yen Ling Chiu** *(National Taiwan University of Science and Technology, Taipei City, Taiwan)*, Microplasma-Enabled Nanoheterostructures for SERS Detection of Aβ Oligomers in Alzheimer's Diagnosis	**#314, Nicolás Coca López** *(Instituto de Catalisis y Petroleoquimica, CSIC, Spain)*, Process Control of Zeolite Synthesis Using {in line} Raman Spectroscopy: A Comparison with {Off line} X-Ray Difraction Analysis	**#433, Guillermo Lopez Reyes** *(University of Valladolid, Spain)*, Real-time Raman detection and quantification of molecular gases at ppm level using hollow-core fiber sensors	**#187, Marek Procházka** *(Charles University, Czech Republic)*, PEDOT:PSS Conducting Polymer Substrates: A Robust Platform For Highly Sensitive Surface-Enhanced Raman Scattering (SERS) Spectroscopy	**#143, Panchali Saha** *(TMC-ACTREC, India)*, Serum Raman Spectroscopy for Oral Disease Stratification
12:00-12:15	**#403, Kacper Jędrzejewski** *(University of Warsaw, Poland)*, EC-SERS Studies of Chloramphenicol on Nanostructured Gold – Control of Adsorption, Redox Transformation and SERS Signal Enhancement	**#47, Olena Zavorotynska** *(University of Stavanger, Norway)*, Insights into synthesis of metal-organic-frameworks (MOFs) with combined in situ approach: Raman scattering, X-ray absorption and X-ray diffraction	**#142, Tim Batten** *(Renishaw PLC, United Kingdom)*, Multimodal characterisation of Li-based battery materials using in situ Raman and SEM analysis	**#15, Saba Bashir** *(University of Montreal, Canada)*, Integrating Machine Learning with SERS Optophysiology for Enhanced Neurotransmitter Sensing	
12-15-12:30	**#24, Raju Botta** *(National Electronics and Computer Technology Center (NECTEC),Thailand)*, Cost-Effective Plasmonic SERS substrate via Tunned Silver Mirror Reaction for Sensitive Herbicide Detection	**#291, Nasim Zarrabi** *(National Physical Laboratory, United Kingdom)*, Metrological Calibration of Raman Shift for Strain Quantification in 4H-Silicon Carbide	**#93, John Kerr** *(University of Bath, United Kingdom)*, Chirality Conferral Enables the Observation of Hyper-Raman Optical Activity		

Scientific Programme

27 August 2026, Thursday

12:30-13:30	**LUNCH**				
	HALL 1 (Plantry/Geo/Materials) Chair: Omer Aydin	**HALL 2 (TC/Imaging) Chair: Mehmet Kahraman**	**HALL 3 (Materials) Chair: Sangwoon Yoon**	**HALL 4 - (SERS/TERS) Chair: Agnieszka Kaminska**	
13:30–13:50	**Invited:** **Miroslav Haluska** (ETH Zurich, Switzerland) "Dual Role of Raman Spectroscopy in Nanosensor Fabrication: Monitoring and Laser Processing of Carbon Nanotubes"	**Keynote:** **Yukihiro Ozaki** *(Kwansei Gakuin University, Japan)*, "Recent Progress on Semiconductoer-enhanced Raman Scatteing"	**Invited:** **Jihyeon Yeom** (KAIST, South Korea) "Chiral-Raman and Its Applications"	**Invited:** **Yuika Saito** (Gakushuin University, Japan) "Temporal Fluctuations in SERS Signals Revealed by DBSCAN-Based Cluster Analysis"	
13:50-13:55					
13:55-14:10	**#367, Gamze N Ozcan** *(Istanbul Technical University, Turkiye)*, Micro-Raman Based Identification Of Impurities In Antarctic Glacier Ice Cores Supported By IC And ICP-MS Analyses	**#298, Sinje Zimmer** *(Forschungsgemeinschaft Feuerfest e.V., Germany)*, High-Temperature Raman Imaging: Unveiling Mineral Processes in Refractory and Ceramic Materials	**#19, Zeyu Zhang** *(Xiamen University, China)*, In situ Raman Reveals CO2 Assisted Reconstruction of Copper Coordination Polymers Promoting C–C Coupling during CO2 Electroreduction	**#115, Taeyeong Kim** *(Korea Advanced Institute of Science and Technology, South Korea)*, Hemispherical gold nanoshell arrays on silicon nanospheres for single-digit nanogap SERS substrates	
14:10-14:25		**#400, Oliviero Cannelli** (*DESY, Germany)*, Controlling Electron-Phonon Coupling via Ultrashort Core-Resonant X-ray Pulses	**#215, Iuliana-Cornelia Sandu-Poplăcean** *(Babeș-Bolyai University, Romania)*, Pigment Diversity and Unusual Blue Biogenic Shell in the Invasive Population of Rapana venosa Sea Snail Revealed by Multi-Laser Raman, SERS, FT-IR, XRD, and SEM-EDX Analysis	**#148, Rasmus Öberg** *(Swedish Defence Research Agency (FOI), Sweden)*, Selective SERS detection of nerve agents using oxime-based Raman probe molecules	
14:25-14:40	**Invited:** **Guillermo Lopez-Reyes** *(Universidad de Valladolid, Spain)* "Raman Laser Spectrometer (RLS) operations and scientific performance for the Rosalind Franklin Mission to Mars"	**#226, Konstantinos Stergiou** *(Lightnovo ApS, Denmark)*, Overcoming Precision Limits in Raman Spectroscopy: A Validated Strategy for Fast and Accurate Dual Axis Calibration	**#347, Raquel Portela** *(Instituto de Catalisis y Petroleoquimica, CSIC, Spain)*, Raman Assessment of Microplastic Production, Identification and Biotransformation during Human Gastrointestinal Digestion	**#426, Ting Wang** *(Vrije Universiteit Amsterdam, Netherlands)*, Lock-in sampling: a time-domain strategy for high-speed widefield SERS imaging	
14:40-14:45					
14:45-15:00	**Invited:** **Michael Gensch** (German Aerospace Center, Berlin, Germany) Time-Domain (Raman) Spectrometers: an emerging ultra-compact and robust class of instruments for Space Exploration	**#497, Natalie Belsey** *(National Physical Laboratory, United Kingdom)*, Visualization of topical drug delivery with label-free chemical imaging	**#516, Zeynep Cantürk** *(Middle East Technical University, Turkiye)*, Improving SERS Sensitivity Using Metal Nanoparticles in Textured Silicon Cavities	**#379, Lars Dannenberg** *(Humboldt-Universität zu Berlin, Germany)*, SERS of stable radicals and Plasmonically Controlled Radical-Mediated Polymerizations	
15:00-15:05					
15:05-15:20	**#248, Maria Fernanda Munoz** *(National Institute of Standards and Technology, MD, USA)*, Validation of Helicity-Resolved Raman Spectroscopy Using Chiral Testing Materials		**#360, Miriam Unger** *(Photothermal Spectroscopy Corp. GmbH, Germany)*, Advancing Polymer Characterization with Simultaneous Optical Photothermal IR and Raman Micro-Spectroscopy	**#307, Kuo Zhan** *(University of Oulu, 90220 Oulu, Finland)*, Deep Learning Analysis of Individual DNA Dynamics on a nanoparticle by Single-Molecule SERS Spectra	
15:30-17:30	CLOSING CEREMONY				

POSTERS

24 August 2026			
#	Topic	Title	Presenter
12	Novel Approaches	Development of broadband multiplex coherent anti-Stokes hyper-Raman scattering (CAHRS) spectroscopy	Kazuki Inoue
23	Materials	Evaluation of spatially offset Raman spectroscopy for depth-selective analysis of highly scattering (layered) paint systems in cultural heritage	Merel C. Konings
25	Coherent Raman Imaging	Instrumentation for super-broadband stimulated Raman scattering spectroscopy and imaging	Jin Guo
59	Materials	Micro-Raman Spectroscopy as a Probe of Magnetic Phase Segregation in Thermally Treated Cr_2O_3-Coated Steel	Giulia Spaggiari
69	Materials	Analysis of Composition-Independent Local Strain in SiGe/Si Superlattices Using Raman Spectroscopy	Hyuksang Kwon
81	Coherent Raman Imaging	Lipid Unsaturation During Dendritic Cell Maturation Revealed by Multiplex CARS Microscopy	Kirin Yasuzaki
95	Materials	Advancing Geochemical Characterisation Through Confocal and 3D Raman Microscopy	Iona Elizabeth Hill
97	Novel Approaches	VibSpecDB: a FAIR-oriented infrastructure for Raman and IR spectroscopy data	Darina Stefaniuk
98	Biology/Biomedicine	Raman Profiling Reveals LRG1-Dependent Shifts in CAF-Linked Biochemical Features in PDAC	Ye Lin Yang
100	Materials	Spatially Resolved Raman Spectroscopy of Janus Monolayers	Eunsung Lee
108	Materials	Interlaboratory Comparison for Determining the Number of Graphene Layers and Characterizing Graphene Powders Using Raman Microscopy	Alessio Sacco
137	Materials	Resonance Raman study of differing electronic transitions in acceptor-donor-acceptor compounds	Sana Maroof
140	Biology/Biomedicine	Raman Spectroscopy and AFM Reveal LRG1 Dependent Biochemical and Mechanical Remodeling During Hepatic Stellate Cell Activation	Gahi Hong
141	Biology/Biomedicine	Raman Spectroscopic Analysis of Microplastic–Cellular Interactions	Jiho Park
150	Biology/Biomedicine	Synthetic Melanin as a Bioinspired Antioxidant: Raman Spectroscopic Validation of Redox Protection in Human Skin	Mohamed Touhid Patel
154	Novel Approaches	Minimum Information About Chemical Investigation (MIChI) For Raman Assays	Noura Rayya
175	Biology/Biomedicine	Non-destructive qualitative analysis of locusts using Raman spectroscopy: A novel, non-invasive method for species identification, biochemical characterization, and pest management applications without sample damage	Anam Zulfiqar
184	Biology/Biomedicine	Raman and Photoluminescence Imaging of Intracellular Localization of PEGylated Carbon Quantum Dots in Stem Cells	Hyunhee Song
192	Materials	Strain-Dependent Raman Signatures of Interlayer Phonons in Few-Layer MoS2	Heesuk Rho
205	Biology/Biomedicine	Advancing SERS based Therapeutic Drug Monitoring for Point of Care Monitoring of Methotrexate	Amalie Løvind Årsten
209	Biology/Biomedicine	Immune Monitoring by Raman Spectroscopy from Acute Inflammation to Stress-induced Dysfunction	Klaudziya Kamiak
232	Biology/Biomedicine	Enhancing Isolate-Level Classification of {Klebsiella pneumoniae} through Data Fusion of Raman and FTIR Spectroscopy	María Gabriela Fernández-Manteca
234	Novel Approaches	The effects of structural evolution on hardness of SiCf/SiC composites studied by In-situ Raman spectroscopy	Guofeng Cheng
240	Biology/Biomedicine	From 5'-GMP To G-Quadruplex: Raman Spectroscopy as a Quantitative Probe of Supramolecular Nucleotide Self-Assembly	Lucia Ďuríšková
245	Biology/Biomedicine	Investigating the Link Between Microplastic Intake and Lung Disease Using Raman Spectroscopy	Emma Smith

POSTERS

24 August 2026

#	Topic	Title	Presenter
249	Biology/Biomedicine	Compact Hybrid SERS Platform Integrating Centrifugal Microfluidics and Automated Sample Preparation for Point-of-Need Therapeutic Drug Monitoring	Roman Slipets
250	Materials	Using In Situ Raman Spectroelectrochemistry to Unveil Active-Species Formation During the Oxygen Evolution Reaction on Doped Nickel Oxide	Jan Ocepek
256	Materials	Interlayer Optical Phonons in Two-Dimensional Moiré Heterostructures	Daekwon Lee
257	Materials	Analysis of Solid Polymer Electrolytes Using PHBHx	Siwoo Kim
292	Theory/Computation	Structural and Vibrational Characterisation of Human Milk Oligosaccharides by Raman, Raman Optical Activity, and DFT Vibrational Calculations	Heber Islas Rios
295	Coherent Raman Imaging	Label-Free Sub-Micron Imaging of Cellulose Microfibrils in {Pseudotsuga menziesii} by Multimodal SHG and CARS Microscopy	Ting Hao Chen
299	Biology/Biomedicine	Crystalline Guanine Formation in Microalgae: Study of Preferred Nitrogen Sources Using Isotopic Labelling and Raman Microscopy	Alexandra Suchá
300	Materials	Recent advances in stable electrodes for two-dimensional materials guided by Raman spectroscopy	Kulurumotlakatla Dasha Kumar
308	Industrial/Societal Applications	Aquatic Aged Micro- Nano Plastic Reference Materials as Resonance Raman-SERRS Traceable Probe for Controlled Exposure and Impact Studies	Simona Pinzaru
312	Non-linear/Time-resolved	A Time-Domain (Raman) Spectroscopy Instrument for Identifying Minerals and Gases in Space Exploration?	Yookyung Ha
316	Biology/Biomedicine	Influence of Tissue Turbidity on Optimal Raman Offset for Transcutaneous Bone Measurement	Joseph O'Halloran
343	Industrial/Societal Applications	Integrated approach based on Raman spectroscopy and chemometrics for the qualitative evaluation of wine and the monitoring of oenological processes	Anna Lisa Gilioli
346	Coherent Raman Imaging	A fiber-compatible fiber optical parametric oscillator for stimulated Raman scattering microscopy	Qingcheng Song
350	Industrial/Societal Applications	Nanostructured SERS Substrates Engineered via Colloidal Lithography for Environmental Nanoplastics Detection	Ioana Cârdan
358	Non-linear/Time-resolved	Structure of the hydrated electron elucidated by the synergy of polarized-resolved FSRS spectroscopy and DFT computations	Marcin Pastorczak
364	Non-linear/Time-resolved	A simple and adaptable solution for measuring time traces from sub-picosecond to sub-microsecond in FSRS spectroscopy	Karolina Skała
376	Materials	Representative Reference Materials for Microplastic Analysis	Nicolas Coca Lopez
377	Coherent Raman Imaging	Cellular Senescence Profiling by Multiplex CARS Spectroscopic Imaging	Ayana Kotegawa
385	Industrial/Societal Applications	Adaptive Confocal Raman Imaging for Rapid Spatial Characterization of Pharmaceutical Solids	Hajar Elazri
387	Biology/Biomedicine	Site-Specific UVRR Investigation of Maltose-Binding Protein Using 5-CN-Trp as a Selective Probe	Wonki Son
388	Industrial/Societal Applications	Online Monitoring of Chemical Processes Using Raman Spectroscopy	Ilyes Bichari
404	Non-linear/Time-resolved	Deep Learning Enhanced Time Domain Raman Spectroscopy	Pietro Lussana
405	Novel Approaches	Automated Single-nanoparticle Raman: Expanding Possibilities Through Increased Data Volume	Mathias Novik Jensen
407	Materials	Decoupling Temperature and Stress in Transferred Silicon Nanomembranes on Heterogeneous Substrates for Elevated-Temperature Applications via Micro-Raman Spectroscopy	Dooyoung Kim
418	Materials	A microfluidic SERS platform for real-time monitoring of antiepileptic drugs	Lydia Federica Gervasini

POSTERS

24 August 2026

#	Topic	Title	Presenter
436	Industrial/Societal Applications	Determination of Methanol in Alcoholic Beverages by Raman Spectroscopy: The Effect of Using Different Internal Standards on Method Performance	Kübra Güven
471	Biology/Biomedicine	Microplastics Monitoring in Human Breast Milk with Raman Microspectroscopy – A Contamination-Free Sample Collection, Preparation and Measurement Approach	Felix Thier
494	Materials	Substrate-Dependent Correlation Between Raman Signatures and Terahertz Conductivity in Single-Layer Graphene	Fatma Feyza Sadıkoğlu
496	Theory/Computation	Piezoelectricity of the β phase of PVDF: investigating the molecular mechanism and the role of intermolecular interactions using density functional theory and Raman spectroscopy	Gianluca Serra
514	Materials	From thermal history to local structure: Raman imaging of NbOx thin films on stainless steel	Céline Eypert
522	Novel Approaches	Coupling Raman Spectroscopy with Electrochemistry for Monitoring DTNB Reduction on a 3D-Printed Electrode	Elif Çalık Kayiş
523	Biology/Biomedicine	Multivariate Spectroscopic Characterization of Canine Cancer: Identification of Molecular Fingerprints	Arti Hole
530	Biology/Biomedicine	High-Throughput Raman-Activated Cell Sorting (HT-RACS) Using Acoustofluidic Chip with Elasto-Inertial Focusing	Gyeong Tae Kim
533	Coherent Raman Imaging	Single-Shot Multiplex SRS: a Platform for Microplastics Detection and Quantification	Federica Padelli
536	Novel Approaches	Toward Single-Particle Raman Microscopy of Vitrified Biological Samples at Liquid Helium Temperature	Polina Kasyanova
537	Novel Approaches	From Raman Spectrometers to Sensors: A New Architecture for High-Resolution Raman Detection	Oliver Lischtschenko
540	Biology/Biomedicine	Monitoring brain tumors by non-invasive, label-free Surface-Enhanced Raman Spectroscopy on biofluids	Salomé Thueler
544	Coherent Raman Imaging	Data-Driven Selection of Raman Signatures for Label-Free SRS Imaging of Lipid Metabolism in HER2-Positive Breast Cancer	Tamás Váczi
554	Non-linear/Time-resolved	Correlative Multimodal Vibrational Imaging with Integrated O-PTIR and PT-SRS for High-Speed Label-Free Chemical Analysis	Miriam Unger
559	Materials	Evaluating picolinamide as a cocrystal former with acidic coformers	Ainur Syeitkhajy
560	Materials	Structural and spectroscopic investigation of isoniazid-based cocrystal systems	Neris Inci Inan
567	Materials	From Co-Crystal to Amorphous Phase and Back: Matrix Isolation Spectroscopy and Computational Investigation of the Reversible Phase Transformation Pathways of the Isoniazid-Gallic Acid System	Dilara Kaplanoğlu
568	Materials	Spectroscopic Evidence for the Formation of a New Prothionamide–Caffeine Crystalline Phase	Merve Durmuş
569	Biology/Biomedicine	Raman Endophenotyping of Fabry Disease: A Framework for Precision Biomarker Discovery	Kübra Telli
571	Materials	Structural Characterization and Thermal Reactivity of Isoniazid-Saccharin Species: From Salts to Adduct	Rezvan Mohammadi
572	Theory/Computation	SSpectrikus: a robust computational framework for stochastic deconvolution and multi-model statistical analysis of vibrational spectr	Bahadır Bozkurt
579	Industrial/Societal Applications	FAIR Analytical Data for Safe and Sustainable by Design	Nina Jeliazkova
582	Industrial/Societal Applications	A Simple and Fast Portable Raman Method for the Identification of Illegal Adulterants in CLA Dietary Supplements through Chemometrics	Sukriye Nihan Karuk Elmas
584	Materials	Optical-Photothermal Infrared (O-PTIR) Microspectroscopy for Simultaneous Submicron Infrared and Raman Analysis of Calcified Materials	Carolin Borbeck

POSTERS

24 August 2026			
#	Topic	Title	Presenter
594	Materials	Understanding Interfacial Charge Transfer Mechanism in Composite Photocatalysts for Enhanced HER Using Raman Spectroscopy	Sulakshana Shenoy

POSTERS

25 August 2026			
#	Topic	Title	Presenter
38	SERS/TERS/Plasmonics	Raman Imaging As A Tool For Evaluating Drug Distribution In Starch-based Orodispersible Films	Francesca Lovati
40	SERS/TERS/Plasmonics	Surface-Enhanced Raman Spectroscopy for Detecting Microplastic-Induced Biochemical Changes in Vigna Radiata Leaves	Hongshu Pu
54	SERS/TERS/Plasmonics	Polarization-Independent Dielectric Metasurfaces for Enhanced Spectroscopy	Jose Francisco Algorri
58	SERS/TERS/Plasmonics	Saliva-Based Surface-Enhanced Raman Spectroscopy For Noninvasive Detection, Typing and Localization of Salivary Gland Tumors	Ida Wiśniewska
62	SERS/TERS/Plasmonics	Comparative Evaluation Of SERS Substrates For Reliable G-Quadruplex Detection	Petra Petrović Popović
89	SERS/TERS/Plasmonics	Bacterial Detection in Wound Infections Using Highly Porous, Flexible and Biocompatible SERS Substrates	David Miguel Henriques Bento
116	SERS/TERS/Plasmonics	Electrochemically-Etched Micro-Macroporous Silicon for SERS Analysis of Complex Samples	Doohong Min
119	SERS/TERS/Plasmonics	Probing Biomolecules Using Surface Enhanced Linear and Nonlinear Raman Scattering	Fariha Binte Rahman
132	SERS/TERS/Plasmonics	Hotspot-Rich, TLC-Integrated Ni@Au/Ag Trimetallic SERS Substrates for On-Site Trace Detection of Explosives, Drugs, and Pesticides	Shashikana Paria
138	SERS/TERS/Plasmonics	Plasmonic Momentum Engineering of Raman Scattering at the Subnanometer Scale	Norihiko Hayazawa
144	SERS/TERS/Plasmonics	Study of Simple Template MIP via LSPR-Raman	Ester Iatta
178	SERS/TERS/Plasmonics	SERS-based Acoustofluidic Platform for Rapid and Sensitive Bacterial Enrichment and Detection	Kyubin Kwon
183	SERS/TERS/Plasmonics	Multimodal sensing of monosaccharides by molecular chirality- and identity-specific SERS responses of aromatic amino acids	Daedu Lee
189	SERS/TERS/Plasmonics	Combined SERS and chemometric analyses of blood plasma and bone marrow towards the pediatric leukemia biomarkers detection	Aneta Aniela Kowalska
190	SERS/TERS/Plasmonics	Structural Characterization of Tel24 On Silver And Gold Nanoparticles Using SERS Spectroscopy	Adriana Kenđel
191	SERS/TERS/Plasmonics	SERS Plasmonic Structure for Biomedical Applications	Ariadna B. Nowicka
218	SERS/TERS/Plasmonics	Flexible Silver-Coated Gold Nanoparticles Loaded Graphene Textiles for Broad-Spectrum In-Situ Detection of Pesticide Residues	Sujia Jiao
221	SERS/TERS/Plasmonics	Towards an Optofluidic Platform for Bioanalysis Based on SERS	Anant Mantha
228	SERS/TERS/Plasmonics	A SERS-Integrated Vertical-Flow Paper Chip with Gold-Coated Cellulose Fiber Substrates for Sensitive Biomarker Detection	Ji Qi
229	SERS/TERS/Plasmonics	Potential-Controlled Binding and Readout in an EC-SERS Aptamer Sensor for Rapid and Sensitive Thrombin Detection	Yujin Cha
231	SERS/TERS/Plasmonics	A Rapid and Highly Sensitive One-Pot Detection Assay for Lung Cancer ctDNA Using a SAW-Enhanced CRISPR-SERS Platform	Mina Shin
280	SERS/TERS/Plasmonics	A Magnet-integrated Paper Chip for On-site Enrichment and SERS Detection of Neglected Tropical Diseases	Mengdan Lu
281	SERS/TERS/Plasmonics	A Molecularly Imprinted SERS Sensor for Label-free Quantitation Whole Exosomes in Biofluids	Jiadong Chen
288	SERS/TERS/Plasmonics	Alginate-based Hydrogel Composites for Surface-Enhanced Raman Spectroscopy Applications	Barbora Štefková
294	SERS/TERS/Plasmonics	Formation of Ag core–Au shell nanostructures with surface-reduction	Yeseul Park
296	SERS/TERS/Plasmonics	Design and Evaluation of Gold-Based Plasmonic Platforms for SERS Detection in Complex Biological Systems	Dragos Ioan Olariu
297	SERS/TERS/Plasmonics	SERS Probing of Biomolecular Interactions of Gold Nanoparticles during Cellular Processing in Co-Cultures	Anastasiia Kniazeva
301	SERS/TERS/Plasmonics	Magnetic Polystyrene Beads Coated with Au and Ag Nanoparticles for SERS Detection of Staphylococcus Aureus Infection and an Alzheimer's Disease Biomarker	Robert Prucek

POSTERS

25 August 2026			
#	Topic	Title	Presenter
330	SERS/TERS/Plasmonics	Silver nanoparticles-environmentaly aged blue polypropylene composite, detection and tracking of micro- and nano- sized plastic particles by SERS	Karlo Maškarić
339	SERS/TERS/Plasmonics	Label-free SERS-based Profiling of Blood Serum Using Differentially Capped Gold Nanoparticles	Septila Renata
366	SERS/TERS/Plasmonics	Influence of Gold Nanoparticle Morphology on SIERS/SERS Enhancement on Silicon Substrates with V-Shaped Microchannels	Italo Odone Mazali
383	SERS/TERS/Plasmonics	Excitation wavelength-dependent variability of methylene blue SERS spectra on silver substrates	Matěj Kmetík
394	SERS/TERS/Plasmonics	Single-Molecule SERS for DNA Nucleobase Classification Using 1D CNN: A Comparative Study with Machine Learning Methods	Enock Adjei Agyekum
410	SERS/TERS/Plasmonics	Controlled Synthesis of Plasmonic Gold Nanostructures for Reproducible SERS Substrates in Biomedical Applications	Ciprian-Paul Măirean
438	SERS/TERS/Plasmonics	Electrochemical SERS of aromatic thiols on silver: potential-dependent study of charge-transfer and molecule–metal interactions	Jakub Havránek
443	SERS/TERS/Plasmonics	In situ Synthesis of Silver Nanoparticles for Surface-Enhanced Raman Spectroscopy-Based Detection of Carbendazim Residues on Apple Surfaces	Sevda Mert
444	SERS/TERS/Plasmonics	Soft Actuator-Based Reconfigurable Platforms for SERS	Görkem Liman
445	SERS/TERS/Plasmonics	Impact of Data Partitioning Strategies on SERS-Based Machine Learning for Reliable Classification of Antibiotic Resistance in Staphylococcus aureus	Zakarya Al Shaebi
446	SERS/TERS/Plasmonics	SERS-Based Spectral Fingerprinting of Brucella in Body Fluids Coupled with Machine Learning	Munevver Akdeniz
451	SERS/TERS/Plasmonics	Cost-Effective SERS Platforms Based on AuNP-Functionalized Carbonized Polyimide for Fluorescence-Suppressed Raman Detection	Sinan Genc
460	SERS/TERS/Plasmonics	Copper Oxide Nanostructures for UV- SERS	Gytaute Sirgedaite
475	SERS/TERS/Plasmonics	SERS-Based Assessment of Salinity in Hypersaline Solutions Supported by Dynamic Light Scattering	Anamaria Couti
477	SERS/TERS/Plasmonics	SERS as a Rapid Quality-Control Tool for Endotoxin Detection in Elastin-like Recombinamers	Marco Veneranda
482	SERS/TERS/Plasmonics	Copper nanoparticles on porous silicon: a new UV-SERS substrate	Ettore Grimaldi
483	SERS/TERS/Plasmonics	Drug Monitoring Via InSitu Methylation And IodideDirected Enhancement	Jianwei Xie
503	SERS/TERS/Plasmonics	Non-aqueous SERS detection enabled by hexadecylamine-capped Ag bumpy nanoshells	Sungjun Kwak
505	SERS/TERS/Plasmonics	Synthesis and performance evaluation of anisotropic silver coated nanoworms for SERS based trace detection of crystal violet and ammonium nitrate	Zeynep Cantürk
509	SERS/TERS/Plasmonics	Background-Free, Label-Free, and Reproducible SERS via Plasma–Halide-Engineered Gold Nanoparticles	Yen Ling Chiu
518	SERS/TERS/Plasmonics	Three-Dimensional Nanostructured Silicon substrate like a Nano-grass Arrays for Surface Enhanced Raman Spectroscopy Applications	Munizer Purica
525	SERS/TERS/Plasmonics	Comparative Study on the Effect of Substrate Structure Type and Laser Wavelength on SERS Performance	Ayse Mine Saridag
527	SERS/TERS/Plasmonics	Comprehensive SERS Characterization of Multi-Class Pharmaceutical Micropollutants	Sylwia Magdalena Berus
528	SERS/TERS/Plasmonics	Surface-Enhanced Raman Spectroscopy in Multi-Omics Integration for Melanoma Profiling	David Lilek
541	SERS/TERS/Plasmonics	Dielectrophoretic trapping and SERS-based detection of micro- and nanoplastics in water	Tomasz Szymborski
542	SERS/TERS/Plasmonics	Advanced Engineering of AuNP-on-AuNF Junctions for Highly Reproducible and Sensitive Induced Surface-Enhanced Raman Optical Activity (SEROA)	Woongil Jeon
547	SERS/TERS/Plasmonics	Antibody-Functionalized Fe_3O_4@Au Magnetoplasmonic Nanoparticles for SERS-Based Bacterial Detection	Rumeysa Polat

POSTERS

25 August 2026			
#	**Topic**	**Title**	**Presenter**
566	SERS/TERS/Plasmonics	Machine Learning-Assisted Deep-UV SERRS for Ultra-Trace Detection and Classification of Nitroaromatic Explosives via in situ Sn-Decorated Aluminum Nanorod Arrays	Lakshay Bhardwaj
589	SERS/TERS/Plasmonics	Probing the competing vibrational Stark effect and interfacial electronic effects in the tunnel junction using tip-enhanced Raman spectroscopy	Ruonan Wang

PLENARY LECTURES

Plenary Lectures

[Abstract:0429]

TERS: Vibrational Spectroscopy and Chemical Imaging on the Nanometer Scale

Renato Zenobi

ETH Zurich

Tip-enhanced Raman Spectroscopy (TERS), introduced in the year 2000, is a nanoscale chemical analysis and imaging method with a spatial resolution down to a few nm, even at ambient conditions [1]. TERS relies on the enhancement of the local electromagnetic field by a plasmonic metal nanostructure that is scanned over the sample by means of a scanning probe microscope, using either AFM or STM feedback. Analogous to SERS, the local electromagnetic field of Raman scattered light is enhanced by many orders of magnitude in TERS. In this fashion, TERS is a variant of scanning probe microscopy that provides localized chemical information.

The working principle, experimental realization, and capabilities of TERS will be introduced [1], with special emphasis on how to avoid artifacts and how to best define the spatial resolution [2].

We will then discuss recent applications of TERS to the spatially resolved chemical analysis and imaging of molecular systems. Examples from recent TERS studies in our laboratory will be chosen, focusing on catalysis [3], biological membranes [4], and the nanostructure of photovoltaic cells [5].

References:

[1] T. Schmid, L. Opilik, C. Blum, and R. Zenobi, Angew. Chem. Int. Ed. 52, 5940-5954

(2013); F. Shao and R. Zenobi, Anal. Bioanal. Chem. 411, 37-61 (2019).

[2] R. Zenobi, N. Kumar, and P. Verma, Nano Lett. 25, 3707-3716 (2025).

[3] Z.-F. Cai, T. Käser, N. Kumar, and R. Zenobi, J. Phys. Chem. Lett. 13, 4864-4870

(2022); Z.-F. Cai, J.P. Merino, W. Fang, N. Kumar, J.O. Richardson, S. De Feyter, and R. Zenobi, J. Am. Chem. Soc. 144, 538-546 (2022); Z.-F. Cai, N. Kumar, and R. Zenobi, CCS Chemistry 5, 55-71 (2023).

[4] Y. Pandey, N. Kumar, G. Goubert, and R. Zenobi, Angew. Chem. Int. Ed. 50, 19041-

19046 (2021); Y. Pandey, A. Ingold, N. Kumar, and R. Zenobi, Nanoscale 16 (2024)

10578-10583. C. Xu, T. Käser, N. Kumar, and R. Zenobi, J. Phys. Chem. Lett. 15, 10237-10243 (2024).

[5] S. Bienz, G. Spaggiari, D. Calestani, G. Trevisi, D. Bersani, R. Zenobi, and N. Kumar, ACS Appl. Mater. Interf. 16, 14704-14711(2024).

Keywords: Tip-enhanced Raman Spectroscopy, Nanoscale Chemical Imaging, Spatial Resolution

Plenary Lectures

[Abstract:0573]

Engineering Sensitivity and Selectivity in Raman Cellular Imaging: Advanced Illumination and Cryogenic Strategies

Katsumasa Fujita

Department of Applied Physics, The University of Osaka, Suita, Japan

Raman microscopy provides label-free molecular imaging of biological systems but is often limited by the weak nature of Raman scattering. Rather than relying solely on improvements in optics and detectors, we have explored strategies to engineer Raman signal generation through spatial, temporal, and spectral control of excitation. Spatial selectivity is achieved using side-illumination approaches, including Bessel-beam and light-sheet excitation, which reduce out-of-focus background and improve sensitivity in three-dimensional tissue and cellular imaging. Temporal control is introduced through rapid cryogenic fixation and cryo-Raman microscopy, enabling preservation of transient cellular states and extended signal acquisition with reduced photodamage. Spectral selectivity is further enhanced by wavelength-controlled excitation, demonstrated through resonance Raman imaging of cellular cytochromes. These approaches illustrate how advanced illumination and cryogenic strategies can expand the sensitivity and molecular selectivity of Raman cellular imaging.

Keywords: Raman imaging, side illumination, rapid freezing, cryo-imaging, resonant Raman scattering

Plenary Lectures

[Abstract:0565]

Impact of Artificial Intelligence in Raman Spectroscopy in Basic Research and Societal Applications

Siva Umapathy

Indian Institute of science, Bangalore, 560012, India

Raman spectroscopic data of complex biological and materials systems are rich in biochemical information thus the spectral datasets are high dimensional with subtle inter-class variations, and often involve a large number of sample categories that conventional chemometric methods struggle to resolve with high accuracy. Artificial intelligence (AI) and deep learning frameworks address these limitations by performing automatic feature extraction, handling nonlinear spectral relationships, and delivering robust classification. This talk presents a body of work from our laboratory demonstrating the impact of AI-driven Raman spectroscopy across basic research and real-world societal challenges.

In materials science, we demonstrate that deep learning architectures like LeNet, ResNet, and Convolutional Autoencoders when coupled with Raman spectroscopy can classify porous bio-carbons derived from nitrogen-rich biomass precursors with accuracies exceeding 92%, enabling rapid quality monitoring and process control in sustainable carbon materials manufacture relevant to CO_2 capture applications. We have also shown that genomic DNA extracted from phylogenetically similar pathogenic bacteria carries unique Raman signatures that reflect differences in nucleobase composition and DNA backbone conformation. A CNN model built on the LeNet architecture achieves 96.33% accuracy in discriminating all 15 bacterial DNA samples. Similarly, we present a culture-independent Raman micro-spectroscopy workflow for identifying ESKAPE pathogens, which are the leading causative agents of hospital-acquired infections, directly from clinical isolates. A deep transfer learning ResNet model trained at the single-cell level achieves 99.99% classification accuracy across all eight species, with robust performance validated on blinded clinical datasets containing both cultured and non-cultured bacterial isolates. Finally, addressing the urgent need for rapid viral disease diagnosis, we report a blood plasma-based Raman spectroscopic approach employing Generative Adversarial Networks to distinguish between seasonal flu, COVID-19, and dengue with predictive F1 scores of 0.96, 0.98, and 1.0 respectively, from a single drop of blood plasma collected from clinical cohorts. Infections by different viruses trigger distinct biochemical changes in plasma proteins, lipids, and nucleic acids, and these changes manifest as subtle differences in the Raman spectral profiles. This demonstrates the potential of AI-enabled Raman spectroscopy as a rapid, reagent-free, and point-of-care screening tool applicable during pandemic outbreaks and in resource-limited healthcare settings.

Keywords: materials, artificial intelligence, biomedical, blood plasma, pathogens

Plenary Lectures

[Abstract:0575]

Engineering Plasmonic Nanostructures For Next-Generation SERS-Based Detection

Isabel Pastoriza Santos

CINBIO, Universidade de Vigo, Vigo, Spain

The physical chemistry of plasmonic nanomaterials provides a powerful framework for linking nanoscale structure–property relationships with advanced Raman-based sensing technologies addressing pressing societal challenges. In this lecture, I will highlight how rationally designed plasmonic nanostructures—both achiral and chiral—enable enhanced light–matter interactions that can be exploited for highly sensitive and selective detection. Particular attention will be devoted to SERS as a versatile platform for (bio)sensing and imaging. I will present recent advances in SERS-based lateral flow immunoassays, demonstrating how plasmonic nanomaterials can push detection limits to the ultrasensitive regime for targets such as SARS-CoV-2 and clinically relevant allergens. In addition, I will discuss the development of plasmonic nanoprobes for multiplex immunophenotyping, enabling the simultaneous detection of multiple biomarkers with high specificity. Finally, I will show how the introduction of chirality in plasmonic nanostructures opens new opportunities for enantioselective SERS detection of biologically relevant molecules, providing additional selectivity dimensions in complex analytical environments.

Keywords: Plamonic nanostructures, chiral nanostructures, sensing, SERS, lateral flow immunoassays

Plenary Lectures

[Abstract:0598]

Plasmonic Porous Materials and Their Applications in SERS

Ramon Alvarez Puebla

ICREA, Passeig Lluís Companys 23, 08010 Barcelona, Spain Departamento de Quimica Fisica e Inorganica; Universitat Rovira i Virgili, Avda. Països Catalans 26, 43007 Tarragona, Spain

Surface-enhanced Raman scattering (SERS) offers exceptional molecular sensitivity, chemical specificity, and the possibility of monitoring chemical and biological processes under realistic conditions.[1] However, the performance of SERS substrates depends not only on their plasmonic response, but also on their capacity to capture, concentrate, transport, and selectively accommodate target molecules. In this context, porosity provides a powerful structural parameter for integrating molecular accessibility and analyte enrichment with electromagnetic field enhancement.[2]

This lecture will examine the design of plasmonic porous materials in which surface area, pore dimensions, adsorption properties, and molecular diffusion are engineered together with the optical response of the metallic nanostructure. Intrinsically porous plasmonic architectures can generate a high density of electromagnetic hot spots while increasing the number of accessible adsorption sites. Complementary hybrid approaches, combining plasmonic nanostructures with polymers, metal–organic frameworks, mesoporous silica, or titania, introduce additional chemical, thermal, mechanical, magnetic, and catalytic functionalities.[2–4]

Particular attention will be given to mesoporous silica and MOF plasmonic systems, where controlled pore networks enable molecular-size selection, analyte concentration, surface functionalization, and diffusion toward SERS-active regions. These properties have supported applications ranging from encoded particles and multiplexed diagnostic assays to intracellular and spatially controlled sensing, as well as the real-time monitoring of chemical reactions.[2,5] Porous plasmonic materials can also act as optically addressable nanoreactors, coupling local electromagnetic enhancement with molecular transport and thermal or catalytic activity. More recent hybrid systems extend these concepts toward the operando characterization of energy-related catalytic processes and the identification of reaction intermediates.[6]

By connecting pore architecture, surface chemistry, plasmonic hot-spot distribution, and molecular dynamics, this lecture will present porous plasmonic materials as multifunctional platforms for analytical sensing, biomedical diagnostics, reaction monitoring, and energy conversion.

References

[1] X. Y. Ling and R. A. Alvarez-Puebla, "Developments of SERS: From Fundaments to Applications," Advanced Materials Interfaces 12 (2025), 2500451. DOI: 10.1002/admi.202500451.

[2] M. A. Correa-Duarte, I. B. Becerril-Castro, and R. A. Alvarez-Puebla, "The Role of Porosity in SERS," Advanced Optical Materials 13 (2025), e01376. DOI: 10.1002/adom.202501376.

[3] E. Tiryaki, T. Zorlu, and R. A. Alvarez-Puebla, "Magnetic–Plasmonic Nanocomposites as Versatile Substrates for Surface-Enhanced Raman Scattering (SERS) Spectroscopy," Chemistry—A European Journal 30 (2024), e202303987. DOI: 10.1002/chem.202303987.

[4] T. Zorlu, I. B. Becerril-Castro, B. Puértolas, V. Giannini, M. A. Correa-Duarte, and R. A. Alvarez-Puebla, "Yolk-Shell Nanostars@ Metal–Organic Frameworks as Molecular Sieves for Optical Sensing and Catalysis," Angewandte Chemie International Edition 62 (2023), e202305299. DOI: 10.1002/anie.202305299.

[5] I. B. Becerril-Castro, V. Salgueiriño, M. A. Correa-Duarte, and R. A. Alvarez-Puebla, "Nano/Micromotor-Driven SERS for Highly

Sensitive and Spatially Controlled Sensing," Advanced Functional Materials 34 (2024), 2314084. DOI: 10.1002/adfm.202314084.

[6] Y. Negrín-Montecelo, A. Sousa-Castillo, N. Cardeñoso-Garrido, L. Guillade, L. V. Besteiro, M. Vázquez-González, R. A. Alvarez-Puebla, B. Puértolas, and M. A. Correa-Duarte, "Plasmon-Driven Nitrogen Photoreduction to Ammonia Using Silica-Encapsulated Au Nanostar/TiO_2 Nanohybrids," Advanced Energy Materials 15 (2025), 2501526. DOI: 10.1002/aenm.202501526.

Keywords: Plasmonic porous materials, applications, SERS

[Abstract:0548]

Raman Spectroscopy for Energy Interfaces and Catalysis

Emiliano Cortes

Nanoinstitute Munich, Faculty of Physics, University of Munich (LMU)

Understanding energy flow across functional interfaces is essential for advancing sustainable technologies in catalysis, solar energy conversion, and energy storage. These interfaces often involve coupled processes - light absorption, charge transfer, molecular adsorption, structural dynamics, and chemical reactivity - that occur across nanometric length scales and under operating conditions.

In this talk, I will discuss how Raman spectroscopy, and particularly surface-enhanced Raman spectroscopy (SERS), can reveal the molecular mechanisms that govern catalytic, reactive, optically active, and hybrid energy interfaces. Since its discovery in 1974, SERS has evolved into a powerful tool for detecting adsorbates, intermediates, catalyst restructuring, and reaction pathways with high sensitivity and spatial resolution. These capabilities make Raman-based methods uniquely suited to follow how interfaces transform light, electrical energy, and chemical potential into molecular function.

Examples will include plasmonic, photonic, photocatalytic, and hybrid nanomaterials for solar-driven reactions such as H_2 evolution and CO_2 reduction, as well as systems where Raman and SERS uncover charge-transfer processes, adsorbate–surface interactions, plasmon damping, and light-induced enhancement mechanisms. I will also highlight complementary imaging and spectroscopic approaches that extend this view to broader classes of energy materials.

Raman spectroscopy helps us see, understand, and ultimately steer energy interfaces for more efficient and scalable technologies.

Keywords: Catalysis, Energy, Interfaces, Raman, SERS, Plasmonics

Plenary Lectures

[Abstract:0259]

In-Situ Raman Probing Surface Reactions

Jian-Feng Li

Department of Chemistry, Xiamen University, Xiamen 361005, China

Understanding the fundamental reaction mechanisms and structure-activity relationships at electrochemical interfaces is essential for advancing electrochemistry and surface catalysis. Such fundamental understanding is strongly dependent on the surface molecular information of the species at the catalytic interfaces, especially that acquired under working conditions. Surface-enhanced Raman spectroscopy (SERS) can provide such information with ultrahigh surface sensitivity. However, only a few metals (such as Au, Ag, and Cu) with specific nanostructures can generate strong SERS effects. This material and morphology limitation has greatly hindered the applications of SERS in probing electrochemical reactions.

To overcome the long-standing limitations, we developed various strategies, including the "borrowing" strategy, shell-isolated nanoparticle-enhanced Raman spectroscopy (SHINERS), and SHINERS-satellite strategy, through the fabrication of plasmonic core-shell nanostructures, allowing in-situ SERS studies at electrochemical interfaces. Using these strategies, the dynamic processes of electrocatalytic reactions, such as the oxygen reduction reaction (ORR), hydrogen evolution reaction (HER), and CO2 reduction reaction (CO2RR), etc., occurring on model single-crystal surfaces or practical nanocatalysts have been systematically investigated. Direct spectroscopic evidence for key intermediates, such as *OH, *OOH, and *O2-, as well as interfacial water structure, has been obtained during reactions, which are combined with theoretical simulations to uncover reaction mechanisms and structure-activity at the molecular level.

To reveal the highly heterogeneous local external fields, we also developed an ultra-high spatial-resolution "molecular ruler" technique, achieving precise measurements of optical, electric, and thermal field distributions at the surface with a spatial resolution of ~2 Anstrom.

References

[1] J. F. Li, Z. L. Wang, Z. Q. Tian et al. Nature, 2010, 492, 392-395.

[2] Y. H. Wang, F. Pan, J. F. Li et al. Nature, 2021, 600, 81-85.

[3] J. C. Dong, J. Feliu, J. F. Li et al. Nat. Energy, 2019, 4, 60-65.

[4] C. Y. Li, Y. Luo, J. F. Li et al. Nat. Nanotechnol. 2020, 15, 922-926.

Keywords: In-situ, Raman spectroscopy, electrochemistry, reaction intermediates

KEYNOTE LECTURES

Keynote Lectures

[Abstract:0014]

Atomistic Modeling of Raman Spectra in Complex Environments: From Solutions to Surface-Enhanced Raman Scattering

Chiara Cappelli

Scuola Normale Superiore, Pisa, Italy

This contribution provides a perspective on the key physicochemical ingredients required for an accurate computational description of Raman and Resonance Raman spectra in complex environments. We discuss the main theoretical challenges associated with achieving a balanced quantum mechanical description of the molecular target, the consistent incorporation of target–environment interactions into the Hamiltonian, and the explicit treatment of strong, specific interactions such as hydrogen bonding. Particular attention is devoted to the role of dynamical sampling of the solute–solvent phase space, which is essential to capture environmental heterogeneity and its impact on vibrational signatures. We also address the inclusion of plasmonic effects within atomistic and multiscale frameworks for the simulation of Surface-Enhanced Raman Scattering (SERS). Through selected applications ranging from solvated molecules to plasmonic nanostructures, we illustrate how these factors critically influence Raman signals.

Keywords: Atomistic modeling, Raman and Resonance Raman, SERS, Aqueous solutions, QM/MM

[Abstract:0086]

Time-Domain (Raman) Spectrometers: an Emerging Ultra-Compact and Robust Class of İnstruments for Space Exploration

Michael Gensch

DLR Institute of Space Research, German Aerospace Center, Berlin, Germany

This work is motivated by the emergence of robust, space-qualified femtosecond lasers and by the fact that time-domain detection allows the design of very compact, robust instruments. As is demonstrated, Time-Domain Raman Spectroscopy (TDRS) enables to measure the same vibrational fingerprint spectrum as conventional Frequency-Domain Raman Spectroscopy (FDRS) while avoiding problems such as fluorescence or ambient light backgrounds. TDRS moreover allows to replace bulky opto-mechanical components and complex detector designs (e.g. CCD or CMOS detector arrays) by a comparatively simple stroboscopic pump-probe scheme at one wavelength in the near-infrared. An additional advantage is the possibility to combine a Time-Domain Raman instrument with a compact THz Time-Domain Spectrometer with very little extra effort. Hence the envisioned final instrument design would combine the virtues of a conventional Raman and FTIR spectrometer in one instrument. A bandwidth of more than 1000 cm^-1 (30 THz) has been recently demonstrated [1,2]. Benchmarking of the existing breadboard models and progress of the work is presented. The timeline to a first demonstrator with technological readiness level 4 is outlined.

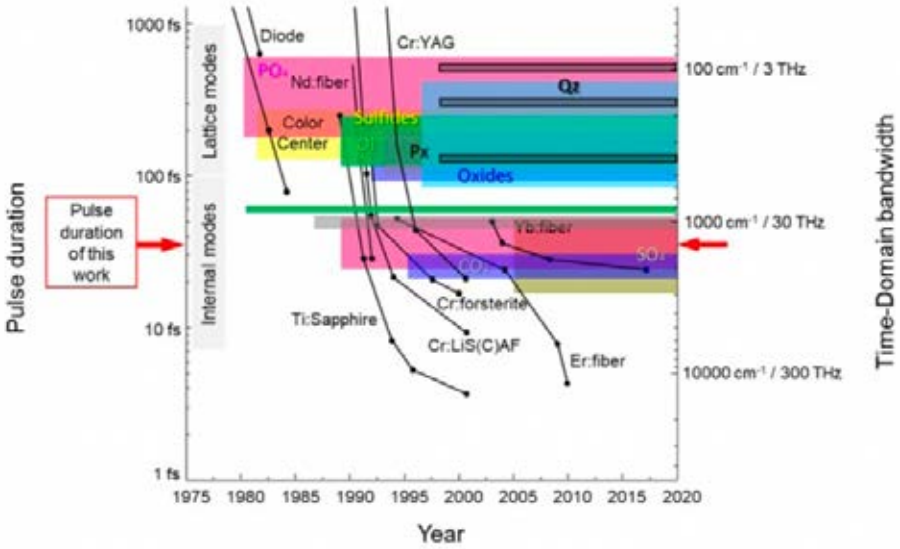
References:

[1] Y. Ha, S. G. Pavlov, M. D. Rabasovic, et al., " Time-Domain Raman Spectroscopy: An Emerging Technique in Space Exploration?," Journ. Raman Spectrosc. 56, 916 (2025).

[2] O. Gueckstock, N. Stojanovic, Y. Ha, et al. "Radiation hardness of ultrabroadband spintronic terahertz emitters: En-route to a space-qualified terahertz time-domain gas spectrometer.," Appl. Phys. Lett. 124, 141103 (2024).

Keywords: Raman, Space Exploration, Time-Domain, Femtosecond Lasers, Minerals, Gases

Figure 1



Evolution of pulse durations of solid-state laser systems since 1975. The corresponding spectral bandwidth in time-domain detection is also shown. Ranges of selected relevant vibrational eigenfrequency classes in planetary materials are also displayed (Qz, quartz; PO4, phosphates; SO4, sulfates; CO3, carbonates; Px, pyroxenes; Ol, olivine). Figure taken from [1] and originally adapted from F. X. Kärtner, E. P. Ippen, and S. T. Cundiff, Femtosecond Optical Frequency Comb: Principle, Operation, and Applications, eds. J. Ye and S. T.Cundiff (Springer, 2006): 54–77.

[Abstract:0217]

Rapid and Sensitive Pathogen Screening Using SERS Sensors

Jaebum Choo

Chemistry, Chung-Ang University, Seoul, South Korea

Rapid and accurate detection of bacterial and viral pathogens is critical for timely clinical decision-making. Traditional culture methods are slow, and RT-PCR requires complex procedures and centralized laboratory facilities, making it less suitable for point-of-care applications. We developed a portable, lysis-free, and ultrasensitive SERS-based platform that integrates two detection modules: an acoustofluidic microfluidic system for E. coli detection and a CRISPR/Cas13a-assisted dual-pathway lateral flow assay (LFA) for viral RNA analysis. In the bacterial module, SERS-tagged E. coli cells are acoustically focused within a microchannel and detected using laser Raman spectroscopy, achieving a limit of detection of 10^4 CFU/mL within less than 1 hour, without the need for cultivation or cell lysis. In the viral module, a five-layer dualpathway LFA couples CRISPR-mediated RNA cleavage with SERS readout, providing 80-fold higher sensitivity and reducing assay time by 10 minutes compared with conventional fluorescence assays, while maintaining RTPCR-level accuracy. This nanoplasmonic SERS platform enables rapid, highly sensitive, and field-deployable detection of bacterial and viral pathogens without requiring genetic extraction, culture, or lysis steps.

Keywords: SERS, diagnostics, pathogen, microfluidics, lateral flow assay

Keynote Lectures

[Abstract:0223]

Versatility and Applications of Raman Spectroscopy in Bioassays

Young Mee Jung

Department of Chemistry, Kangwon National University, Chuncheon, Korea

Surface-enhanced Raman scattering (SERS) is a powerful platform for ultrasensitive and molecularly specific detection of chemical and biological species. These capabilities have driven broad applications ranging from heavy metal analysis to disease biomarker detection. Recent advances in SERS-based biosensors are rapidly expanding their impact in disease diagnostics. To further improve detection performance, extensive efforts have been devoted to developing strategies that enhance SERS sensitivity.

We have recently reported a variety of SERS-active substrates for biomolecular detection and demonstrated their versatile applications in highly sensitive SERS-based bioassays. In this presentation, recent advances in SERS-based bioassays for biomolecular analysis, highlighting their potential, versatility, and utility in ultrasensitive detection will be introduced.

Keywords: SERS, bioassay, disease diagnosis

Keynote Lectures

[Abstract:0391]

Recent Progress on Semiconductoer-Enhanced Raman Scatteing

Yukihiro Ozaki

School of Biological and Environmental Sciences, Kwansei Gakuin University

In 1982 Yamada et al. succeeded in observing SERS of pyridine on the surface of NiO and TiO2. This might be the first observations of semiconductor SERS. Semiconductor-enhanced Raman scattering was looked again after 2000. For example, B. Zhao cooperated with Lombardi et al. reported semiconductor-enhanced Raman scattering for metal oxides, metal tellurides, metal sulfides, and so on. They proposed a clear CT model to explain the enhanced Raman on semiconductor materials. There are several kinds of semiconductor materials for enhanced Raman scattering. Metal oxides such as TiO2 and ZnO are representative ones. The enhancement factor of semiconductor-enhanced Raman scattering is typically 103-108.

The advantages of semiconductor-enhanced Raman scattering are summarized as follows:

(1) Semiconductor materials have excellent high chemical and thermal stability. Thus, they can avoid the problem of signal reproducibility caused by substrate oxidation.

(2) Semiconductor materials have superb surface modifiability. In contrast to metal materials, most of common functional groups can be directly adsorbed on semiconductor materials surfaces.

(3) Semiconductor materials have good biocompatibility.

(4) Semiconductor materials have a variety of species.

The SERS enhancement mechanisms of semiconductors are concerned both with electromagnetic and chemical enhancement. Metals show LSPR due to high-density of free electrons, on the other hand, the semiconductor materials primarily achieve electromagnetic enhancement through light-trapping and subwavelength-focusing capabilities, as well as morphology-dependent resonances such as Mie resonance.

Keywords: Semiconductor-enhanced Raman Scattering, SERS, Chemical mechanism, Charge-transfer, Mie resonance

Keynote Lectures

[Abstract:0493]

Multifunctional Plasmonic Nanoplatforms for SERS, Bioimaging and Plasmon-Enhanced Therapies

Simion Astilean

Department of Biomolecular Physics, Faculty of Physics, Nanobiophotonics and Laser Microspectroscopy Center, Interdisciplinary Research Institute on BioNanoScience, Babes-Bolyai University, Cluj-Napoca, Romania

Plasmonic nanoparticles have emerged as a central point of multidisciplinary research, driven by the distinct optical signatures of localized surface plasmon resonance - specifically electromagnetic field localization, photothermal conversion, and hot carrier generation. These phenomena, coupled with highly adaptable surface chemistry and enhanced biocompatibility, facilitate the development of multifunctional nanoplatforms for advanced biomedical interventions, such as SERS applications, bioimaging and plasmon-enhanced therapies.

This presentation offers a comprehensive overview of the plasmonic nanoplatforms developed in our laboratory, highlighting their diverse applications in SERS-based sensing, cell bioimaging and plasmonic nanotherapies. Our research follows two distinct fabrication METHODS: first, the colloidal synthesis of gold and silver nanoparticles with tunable morphologies—including nanorods, nanoprisms, and bipyramids—engineered for localized surface plasmon resonance (LSPR) across the visible to near-infrared (NIR) spectrum. Secondly, we present the fabrication of solid SERS substrates and hybrid architectures, integrating graphene oxide (GO) and biopolymers with plasmonic components to achieve multifunctional capabilities and enhanced biocompatibility.

The plasmonic response of the fabricated nanostructures was systematically investigated and correlated with their morphology, surface topography, and composition through a synergistic approach involving experimental techniques (SEM, TEM, DLS) and FDTD-based theoretical modeling. These versatile nanoplatforms served as high-performance optical probes for single-cell spectroscopic investigations, utilizing SERS, localized surface plasmon resonance scattering (LSPR-S), and fluorescence lifetime imaging (FLIM). By employing scanning confocal Raman/SERS microscopy in tandem with dark-field and Re-scan fluorescence microscopy, we achieved precise intracellular mapping of nanoparticle localization, chemical interactions, and pH variations. Beyond bioimaging, we demonstrate several 'proof-of-concept' applications for plasmon-enhanced photothermal (PTT) and photodynamic (PE-PDT) therapies, as well as controlled drug delivery systems (doxorubicin, cisplatin). Our work also encompasses the synthesis of gold atomic nanoclusters, demonstrating their versatile utility as highly sensitive components for sensing and imaging platforms. Recently, we utilized graphene oxide-gold nanoparticle platforms (GO-AuNPs) as SERS substrates to investigate DNA detection and hybridization.

Keywords: Plasmonic nanoparticles, SERS applications, Plasmon-enhanced therapies,

Keynote Lectures

[Abstract:0506]

Biochemistry of Lipid Metabolism of Animal Cells as Probed by Surface-Enhanced Raman Scattering

Janina Kneipp

Humboldt-Universität zu Berlin

Raman signals, and also SERS signals from typical vibrations of lipid molecules are often much lower than those of other biomolecular species, such as aromatic amino acid side chains or nucleotides. A main reason is their relatively weak Raman cross section. In live cells, the lipids often remain completely undetected. In the past years, we have worked with different cellular models that enabled us to manipulate the lipid content in living cells, and have shown that lipid structure and interaction in cells can be followed based on their SERS spectra [*ACS Nano, 2019,* 13, 9363-9375; *Analytical Chemistry, 2021,* 93, 10106–10113]. As reference models, we have discussed SERS data of pure liposomes and cell membranes. Based on this, we have more recently established several experimental models to study sphingolipid metabolism, which is controlled by different enzymes. By altering the activity of enzymes that act in the generation and decomposition of ceramide in different metabolic pathways and cellular compartments, we control the ceramide levels in different cell types and can study the according effects by SERS [*ACS Nano, 2026,* 10.1021/acsnano.5c22213]. Here, data from samples will be discussed where enzymes that are responsible for increase and decrease of ceramide levels are inhibited. The molecular changes due to disturbed lipid homeostasis occur with respect to many different parameters and interactions that reveal very specific patterns and co-occurrence. The latter are deduced based on different approaches of machine learning to extract important spectral variables, and to understand their co-occurrence, combined with pure-molecule models, to infer on molecular interactions *in vivo*. The talk will illustrate how the reconstruction of specific molecular interaction patterns by machine learning analysis of vibrational information and 3D ultrastructural data are utilized to probe cellular reactions that are a consequence by the disrupted lipid metabolism.

Keywords: SERS, gold nanoparticles, sphingolipids, enzyme, Random forest

Keynote Lectures

[Abstract:0520]

2D Maerials Under High-Pressure Conditions: Strain Effects on the Phonon Spectrum

Antonio Gomes Souza Filho

Physics Department, Universidade Federal do Ceará, Fortaleza, Brazil

Raman spectroscopy is a powerful technique for investiganting 2D materials because phonons dynamics is very sensitive to enviroment either by doing or strain transfers effects. In this talk, we show how Raman spectroscopy can be used to probe the effects strain in 2D materials by using high-pressure techniques in bilayer, few-layer graphene and WSe_2. Firstly, we show the influence of the substrate and the pressure transmitting medium on bilayer graphene by using a sample where both suspended and partially supported 2D material are probed. The experiments unveiled that charge carrier density saturates quickly at low pressures (2 GPa) while biaxial strain continuously increases with pressure. Secondly, we show how the biaxial strain leads to the formation of 2D diamond-like sp^3 carbon in few-layer graphene stacks at room temperature and pressure of 7 GPa. Thirdly, we present a comprehensive study of the Raman spectra of monolayer WSe_2 under high pressure up to 40 GPa. By using diamond as the substrate, we isolate the intrinsic vibrational response of monolayer WSe_2 from substrate-induced effects. These findings provide practical guidelines for minimizing substrate- and pressure transmiting medium-related artifacts, thus enabling more accurate and reproducible high-pressure Raman characterization of two-dimensional materials.

Keywords: Strain effects, 2D materias, high-pressure

Keynote Lectures

[Abstract:0546]

Electrochemical Tip-Enhanced Raman Spectroscopy--More Than 10 Years Development, Current Status and Future Opportunity

Yi Fan Bao, Mengyuan Zhu, Xiaojiao Zhao, Xiang Wang, Bin Ren

College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, China;State Key Laboratory of Physical Chemistry of Solid Surfaces;Innovation Laboratory for Sciences and Technologies of Energy Material of Fujian Province (IKKEM)

Tip-enhanced Raman spectroscopy (TERS) was invented in 2000, boosting the Raman signal by the localized surface plasmon resonance effect from nanosized silver or gold tips of scanning probe microscopy, including scanning tunneling microscopy and atomic force microscopy. This technique has opened a new era of vibrational spectroscopy, which allows the characterization of surface structures with chemical identities at the nanometer spatial resolution. 15 years after the invention of TERS, TERS was successfully applied in electrochemical systems, realized the so-called electrochemical TERS (EC-TERS) providing unprecedented sensitivity and spatial resolution to understand the solid-liquid interfaces with potential control. This is the 11 years after the report of EC-TERS, and EC-TERS have experienced a leap in terms of the sensitivity, spatial resolution and time resolution.

In addition to an overview of the field, this talk will focus on the current development in my group, in terms of the tip preparation, instrumentation, electrochemical design, as well as artificial intelligent assisted signal augmentation. All these efforts contribute to the significantly improvement capability of EC-TERS, which makes the study of electrocatalytic systems with 2~3 nm spatial resolution. It even allows the simultaneous acquisition of morphological and spectral information, which has never been realized before.

Keywords: Tip-enhanced Raman, electrochemistry, electrocatalysis, instrumentation, tip preparation, AI

[Abstract:0550]

Raman Microscopic Analysis of Cellular Function in Vitro

Hugh James Byrne

Technological University Dublin

The presentation describes ongoing efforts to explore the capabilities of label free vibrational spectroscopy to analyse complex processes in cellular systems, in particular by controlling the variance of the system by external factors such as drug dose, time, and seeding. The rapid emergence of, for example, coherent Raman and multimodal photothermal techniques indicate that the ability to monitor processes at a subcellular level across the vibrational spectrum in real time is imminent, and therefore the challenge of datamining and understanding the relevance signatures is increasing in relevance.

The analysis of spectroscopic signatures of biological systems necessarily involves multiple replicates and/or variants of often physically and chemically complex samples, requiring the implementation of multivariate statistical methods, chemometric and/or machine learning algorithms. Unsupervised analysis explores the intrinsic variance within the sample dataset, while supervised approaches can superimpose a classification requirement or seek to identify co-variance patterns within the dataset and an external parameter. Radiation or drug dose can be employed, for example, to exert some degree of control over the variance, which can then be datamined using linear or nonlinear regression techniques, and thus the parameters can act as indicators of change. In a kinetically evolving system, time itself is an indicator of change and the spectroscopic evolution can be modelled and data mined according to phenomenological rate equation systems. In systems in which multiple components are changing simultaneously, the analysis must be seeded with a prior knowledge of the components, biasing the variance such that they and their evolution can be accurately identified and monitored.

The limitations of the technique in the context of monitoring metabolic processes, and potential routes towards improving datamining techniques are discussed.

Keywords: Cellular Analysis, Data Mining, Kinetic Evolution

[Abstract:0583]

Multi-Excitation Raman Spectroscopy and İts Applications in Biology and Medicine

Sumeet Mahajan

University of Southampton

Raman spectroscopy has been widely used for chemical characterization and analysis. However, its specificity for the analysis of complex environmental or biological samples is low. To address this issue, we have developed a novel spectral-omics or 'spectromics' platform technology called multi-excitation Raman spectroscopy (MX-Raman). The method uses multiple lasers to excite different molecular vibrations in a sample, and the resulting combined data is analyzed resulting in improved specificity and higher analytical performance for classification of biological samples and disease conditions. MX-Raman offers more information than conventional single-excitation approaches by using the (a) dependence of Raman cross-section on wavelength and (b) electronic resonance and pre-resonance excitation along with non-resonant Raman of molecules in a 'complex mixture' such as a biological sample.

In this talk I will provide an overview of our research on the application of MX-Raman to different biological areas, and in particular focusing on dementia or neurodegenerative diseases. I will present our data on the comparison of MX-Raman to conventional single-excitation Raman spectroscopy and describe the analytical performance of the method. I will describe our various clinical studies and share data on the detection of different neurodegenerative diseases and conditions including Alzheimer's disease in different biofluids. I will highlight the interdisciplinary nature of the work and demonstrate how the work is leading to the translation of MX-Raman as an analytical platform for dementia detection and diagnosis.

Keywords: MX-Raman, Multi-excitation Raman, Dementia, Neurodegenerative Diseases, Alzheimer's Disease

Keynote Lectures

[Abstract:0585]

From Raman Fingerprints to Patients: AI-Driven Translational Raman Spectroscopy for Precision Medicine

Juergen Popp[1,2]

[1]*Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich-Schiller-University Jena, Helmholtzweg 4, 07743 Jena, Germany*
[2]*Leibniz Institute of Photonic Technology, Member of Leibniz Health Technologies, Albert-Einstein-Straße 9, 07745 Jena, Germany*

This lecture will present recent advances in translational Raman instrumentation addressing two major unmet medical needs: infection diagnostics and oncology. Although these application areas differ substantially, both share a common challenge: the need for rapid and reliable clinical decision-making. A key enabler for translating Raman spectroscopy into these environments is artificial intelligence (AI), which transforms complex molecular fingerprints into actionable diagnostic information.

The first part of the lecture will focus on infection diagnostics. Sepsis and other severe infections require immediate therapeutic intervention, yet current diagnostic workflows often fail to provide timely information. Raman spectroscopy combined with AI enables rapid molecular characterization at three clinically relevant levels: host-response profiling, pathogen identification, and antimicrobial susceptibility testing. Together, these approaches provide insights into disease severity, infectious agents, and resistance patterns, supporting faster and more individualized treatment decisions.

The second part will address oncology. Clinical translation will be illustrated using Raman-InvaScope, an MDR-compliant fiber-optic Raman platform for in vivo tissue assessment and intraoperative decision support. While point-based Raman measurements provide highly specific molecular information, future surgical guidance requires spatially resolved tissue characterization. Therefore, Raman spectroscopy is increasingly complemented by coherent Raman imaging and additional nonlinear optical contrasts, enabling rapid label-free visualization of tissue morphology and biochemical composition. Combined with recent advances in fiber-optic probe and endoscope development, these technologies are paving the way for real-time image-guided interventions and integrated “see-and-treat” concepts that combine diagnosis and therapy within a single clinical workflow.

Despite the apparent differences between infection diagnostics and oncology, both fields are moving toward the same overarching vision: individualized, data-driven patient models. In the final part of the lecture, the concept of AI-enabled optical digital twins will be introduced. By integrating longitudinal Raman-derived molecular fingerprints with imaging, clinical metadata, and physiological information, digital twins may enable predictive diagnostics, therapy monitoring, and personalized healthcare strategies.

Acknowledgment: Financial support from the EU, the Federal Ministry of Research, Technology and Space Germany (BMFT), the German Research Foundation (DFG), the Carl-Zeiss Foundation, and the Free State of Thuringia is gratefully acknowledged.

Keywords: Raman spectroscopy, artificial intelligence, infection diagnostics, oncology, digital twins

Keynote Lectures

[Abstract:0586]

Extending the Photonic Data Science Toolbox: Data Infrastructure Methods and Physically Inspired Deep Learning Models

Thomas Wilhelm Bocklitz

Friedrich Schiller University Jena, Germany

Within photonic data science tools to store, archive and analyze vibrational spectroscopy data are developed, therefore the research field can be divided into pre-processing and data modelling phases, as well as data/model storage. In spectral measurement methods such as Raman spectroscopy, etaloning distorts spectroscopic data. To address this issue, a two-phase transfer learning strategy [1] has been developed to integrate computational physics with deep learning. This begins with pre-training on over 30,000 simulated spectra, followed by fine-tuning with real data. The extensive simulated dataset improves model generalisation and reduces distortion by up to 70%, thereby enhancing spectral accuracy and interpretability.

Modelling biophotonic data, particularly Raman spectroscopy, presents challenges due to limited spectral data, which can lead to overfitting. This issue is resolved by generating simulated spectra using quantum chemistry methods, which enables the efficient pre-training of deep learning models [2]. These models are then fine-tuned using smaller datasets, such as bacterial Raman spectra. This approach is cost-effective and maintains performance comparable to models trained from scratch. This validates the utility of synthetic data for model pretraining.

Finally, both the model and the data need to be stored reliably. In microscopy research, integrating vast volumes of data from disparate platforms is challenging. Adhering to FAIR data principles necessitates the use of tools that can integrate data from various sources. LEO (Linking Electronic Lab Notebooks with OMERO) addresses this by creating links between distributed systems [3]. Initially designed for electronic laboratory notebooks (ELNs) and OMERO, its scalable architecture now supports broader integration, such as the link with databases like VibSpecDB [4]. This enhances collaboration and data management in photonic data science.

References:

[1] R. Vulchi et al., J. Chem. Inf. Model. 2025, 65, 21, 11733–11745.

[2] J. Kamran et al. J. Chem. Inf. Model. 2025, 65, 13, 6632–6643

[3] Guerrero et al. Arxiv https://doi.org/10.48550/arXiv.2508.00654.

[4] VibSpecDB https://vibspecdb.de/

Keywords: Machine learning, Physics Inspired Deep Learning, Data infrastructure

Keynote Lectures

[Abstract:0591]

Towards Quantitative Analysis of Defects in Tip-Enhanced Raman Spectroscopy of Graphene and Other 2D Systems

Ado Jorio

Physics Deparment, UFMG, Belo Horizonte, Brazil

Different applications of tip-enhanced Raman spectroscopy in two dimensional systems have been demonstrated [1], including contaminations in MoSe2 [2,3], studies on substrate-related optical activity in transition metal dichalcogenide [4], tellurium nanowires of different diameters [5], collagen fibrillogenesis [6] and even the optical properties of cicada wings [7]. While TERS provide enhanced spatial resolution [8], it also brings new challenges related to the inner dependence of the tip-enhancement on several fundamental and instrumental aspects. Based on our recent developments in TERS theory, including coherence and symmetry aspects [9], we provide quantitative analysis for defects and contaminations in 2D systems. We also rationalize the anomalous tip-sample distance behaviour [10] observed in graphene at ambient conditions.

References:

[1] A Jorio, LG Cançado, A Hartschuh. Introduction to the special issue 'Tip-enhanced Raman spectroscopy (TERS9)'. Journal of Microscopy 301 (1), 3-4 (2026)

[2] JE Guimarães et al. Nano-Raman Spectroscopy Figure of Merit and Chemical Analysis of Contaminations in Single-Layer MoSe2, ACS nano 19 (40), 35438-35446 (2025)

[3] JE Guimaraes et al. Noise reduction in nano-Raman spectroscopy using principal component analysis. physica status solidi (b) 263 (1), e202500291 (2026)

[4] R Nadas et al. Substrate-related optical activity in monolayer WS2-WS2 and MoSe2-MoSe2: A tip-enhanced Raman spectroscopy study. Journal of Microscopy 301 (1), 5-11 (2026)

[5] D Sier et al. Nano-Raman Spectroscopy of Tellurium Nanowires. Accepted in Journal of Raman Spectroscopy.

[6] MA Paularie et al. Exploring collagen fibrillogenesis at the nanoscale: Tip-enhanced Raman imaging of protofibrils, Journal of Microscopy 301 (1), 12-19 (2026)

[7] VAF Torres et al. Optical properties of cicada wings covered by graphene studied by nano-Raman spectroscopy. Journal of Microscopy 301 (1), 30-39 (2026)

[8] V Monken et al. Plasmonic Bi-Cavity Nanostructure for Efficient Light Collection and Localization. Accepted in Analysis & Sensing.

[9] R Corrêa, LGCançcado and Ado Jorio. Theory for TERS of 2D materials including out-of-plane Raman response. Submitted.

[10] AG Pereira et al. Anomalous Tip-Sample Distance Behavior on the Tip-Enhanced Raman Spectroscopy of Graphene in Ambient Conditions. Accepted in Applied Physics Letters. arXiv preprint arXiv:2601.14178

Keywords: TERS, two-dimensional systems, graphene, defects, contaminations

Keynote Lectures

[Abstract:0592]

Stimulated Raman Photothermal Microscopy: Chemical İmaging with High Sensitivity and Ease of Operation

Ji Xin Cheng

Boston University, USA

Stimulated Raman scattering (SRS) microscopy has shown enormous potential in revealing molecular structures, dynamics, and couplings in a complex system. Yet, the sensitivity of SRS is fundamentally limited to milli-molar level due to the shot noise and the small modulation depth. Additionally, the operation of SRS imaging is complicated by cross phase modulation and laser noise. We recently revisited SRS from the perspective of energy deposition (Figure 1). The stimulated Raman process pumps molecules to their vibrationally excited states. The thereafter relaxation heats up the surrounding and induces refractive index changes. By probing the refractive index changes with a laser beam, stimulated Raman photothermal (SRP) microscopy is developed [1], where a >500-fold boost of modulation depth is achieved. Moreover, SRP imaging can be operated with a relatively noisy fiber laser for excitation and a long working distance air condenser for signal collection, allowing system design to be much more flexible [2]. In summary, SRP microscopy opens a way to perform bond-selective chemical imaging with ultrahigh sensitivity and ease of operation [3].

Figure 1: As a non-parametric process, stimulated Raman gain (SRG) and loss (SRL) collectively excite the target molecule to its vibrational excited states, which deposits energy onto the sample and generates heat via nonradiative decay on the picosecond time scale. This physics builds the foundation for highly sensitive photothermal detection of a Raman signal.

References:

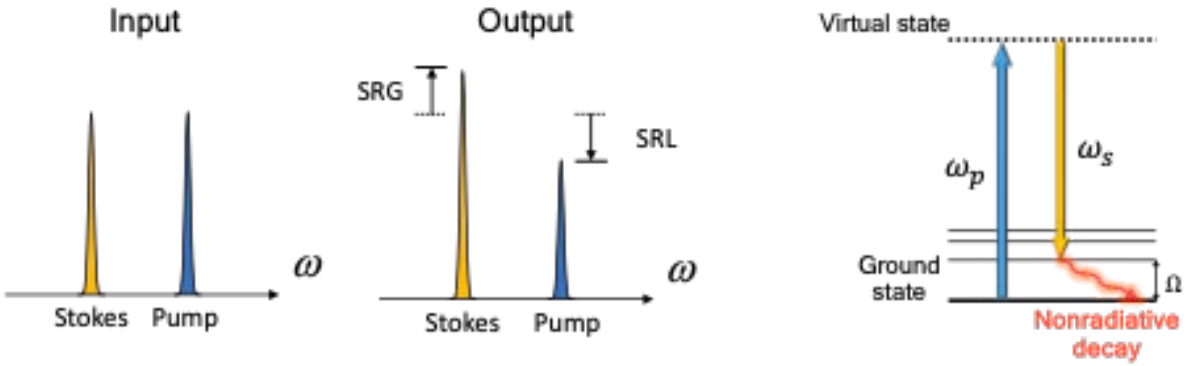
[1] Yifan Zhu, Xiaowei Ge, Hongli Ni, Jiaze Yin, Le Wang, Haonan Lin, Yuying Tan, Chinmayee V. Prabhu Dessai and Ji-Xin Cheng, Stimulated Raman photothermal microscopy towards ultrasensitive Chemical imaging, Science Advances, 2023, 9, eadi2181.

[2] Xiaowei Ge, Yifan Zhu, Dingcheng Sun, Hongli Ni, Yueming Li, Chinmayee V. Prabhu Dessai, Ji-Xin Cheng*, Fiber laser based stimulated Raman photothermal microscopy towards a high-performance and user-friendly chemical imaging platform, PhotoniX, 2025, 6:35.

[3] Yifan Zhu, Xiaowei Ge, Hongli Ni, Ji-Xin Cheng, Stimulated Raman Photothermal Microscopy: Theory and Implementation, Advances in Optics and Photonics, 2026, Vol. 18, page 369. https://doi.org/10.1364/AOP.568778

Keywords: Stimulated, Raman, Photothermal, Microscopy

Figüre



Keynote Lectures

[Abstract:0597]

Vibrational Dynamics À La Carte: Background-Free Mode-Selectivity by Phase-Controlled Impulsive Raman Spectroscopy

Tullio Scopigno

Dipartimento di Fisica, Universitá di Roma "La Sapienza", Italy / Istituto Italiano di Tecnologia, Graphene Labs, Via Morego 30, Genova, Italy

Tracking excited-state vibrational dynamics on femtosecond timescales is fundamental to capturing the primary steps of photophysics and photochemistry. Electronically resonant Impulsive stimulated Raman scattering (ISRS) allows, in principle, to selectively excite desired vibrations and disentangle spectral components arising from different excited states, efficiently retrieving time-dependent dynamics [1-3]. ISRS, however, is systematically hampered by massive transient absorption backgrounds that obscure weak vibrational signatures. While empirical subtraction is possible, the resulting stochastic noise necessitates long acquisition times, often incompatible with irreversible processes or photodegradable samples.

Here, we introduce detection-phase controlled chirp-encoded ISRS, a paradigm-shifting approach that simultaneously achieves intrinsic background cancellation, a dramatic reduction in experimental times and mode-selective enhancement [4]. By leveraging the spectral-to-temporal mapping of a strongly chirped probe, we demonstrate that strategically selecting a pair of pump-probe delays -separated by a specific phase shift relative to the vibrational period- enables the direct "gating out" of non-oscillatory backgrounds. We experimentally validate this protocol on Cresyl Violet, retrieving pure ground- and excited-state vibrational spectra with an unprecedented speedup of over two orders of magnitude (>400x) compared to conventional ISRS. This method bypasses the Nyquist-limited delay scanning and active pump modulation, transforming hours-long measurements into rapid acquisitions. Our results provide a universal, high-throughput strategy for background-free vibrational spectroscopy, overcoming the fundamental limitations of transient absorption backgrounds in complex photo-physical and photo-chemical systems.

References:

[1] L. Monacelli et al. The Journal of Physical Chemistry Letters, 8, 966, (2017)

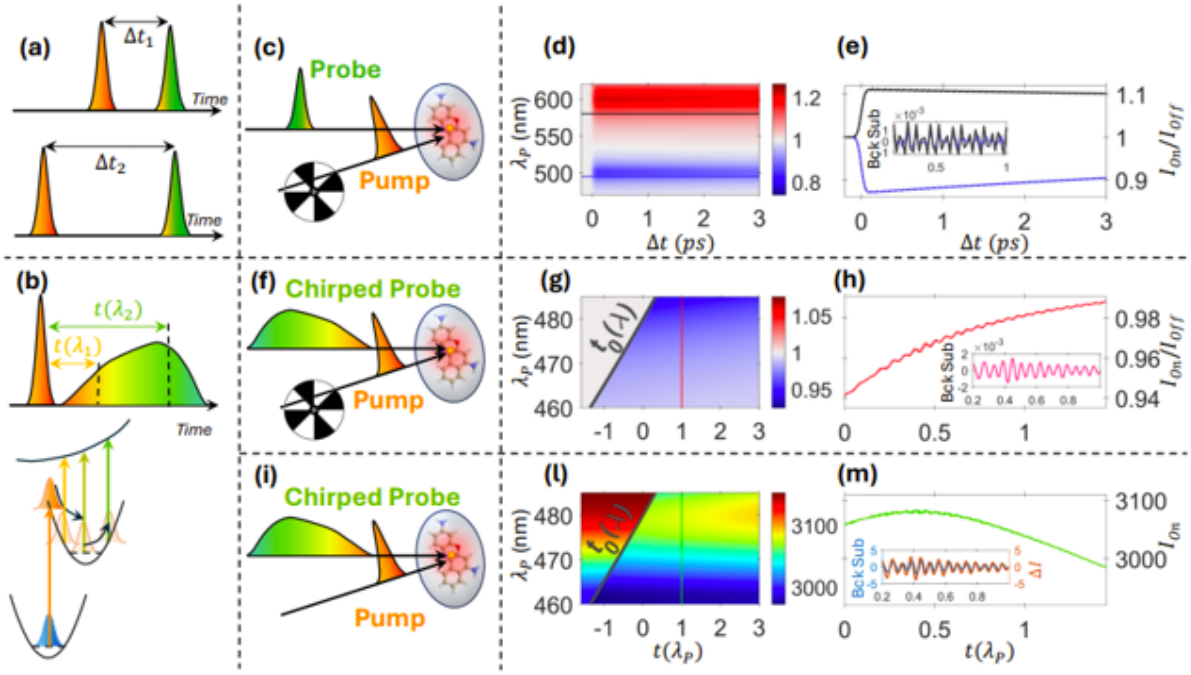
[2] E. Mai et al. The Journal of Physical Chemistry Letters 15, 6634–6646 (2024)

[3] G. Giovannetti et al. Communications Chemistry 9, 57 (2026)

[4] G. Batignani et al. Submitted

Keywords: Background-Free Mode-Selectivity, Phase-Controlled Impulsive, Raman Spectroscopy

Figure 1



Conventional ISRS (a,c,d,e) vs chirped probe ISRS (b). With the latter approach, the differential transmissivity can still be recorded at a fixed Δt by modulating the RP (f-h). Importantly, as the vibrational oscillations are also imprinted onto the transmitted probe spectrum, they can be isolated simply by recording the PP spectrum and removing the probe spectral envelope, without requiring any pump modulation (m), evaluating the difference of two traces separated by a fraction of the vibrational period (40 fs for blue and orange lines in the subplot m, respectively)

INVITED LECTURES

Invited Lectures

[Abstract:0042]

4-Shot, 2-Color Stimulated Raman Histology

***Sandro Heuke*[1], *Gina Benni*[1], *Jitendra Acharyya*[1], *Hervé Rigneault*[1], *Romain Appay*[2]**

[1]*Aix Marseille University, CNRS, Centrale Med, Institut Fresnel, 13013 Marseille, France.*
[2]*APHM, CHU Timone, Service d'Anatomie Pathologique et de Neuropathologie, Marseille, France.*

More than half of the population in industrialized countries will receive a cancer diagnosis, and the majority of solid tumors are treated surgically. A critical challenge during oncologic surgery is identifying tumor margins to ensure complete resection while preserving healthy tissue. Today, this decision relies on conventional histopathology, which requires tissue fixation, sectioning, staining, and expert evaluation—a process that takes at least tens of minutes and typically exceeds 24 hours. As a consequence, surgical guidance is not available, leading to prolonged procedures, repeat surgeries, and compromised patient outcomes.

Stimulated Raman scattering (SRS) microscopy has emerged as a powerful route toward slide-free, label-free histology by providing intrinsic biochemical contrast that correlates with established histopathological features. However, despite its diagnostic promise, current stimulated Raman histology (SRH) implementations remain too slow to meet the throughput demands of intraoperative use. This limitation arises from two fundamental constraints: the need for shot-noise-limited detection in pump–probe SRS measurements and the restricted laser duty cycle imposed by the minimum pulse duration required for adequate spectral resolution.

Here, we present a 4-shot, 2-colour SRH platform that overcomes these limitations through system-level redesign. By operating a shot-noise-limited laser architecture at a reduced repetition rate of 11 MHz—while maintaining picosecond pulse durations required for vibrational specificity—we increase the available SRS signal per pulse. A compact fibre-based optical parametric oscillator provides the second excitation colour at matching repetition rate, enabling robust two-colour imaging under shot-noise-limited conditions. Compared to conventional 80 MHz systems, this approach enables more than an order-of-magnitude reduction in dwell time at constant signal-to-noise ratio.

To remove the remaining speed bottleneck of lock-in-based demodulation, we implement a dual-colour, time-gated boxcar detection scheme. This strategy enables direct extraction of two-colour SRS contrast within four laser shots and an effective integration time of 350 ns.

By combining low-repetition-rate, shot-noise-limited excitation with ultrafast time-gated demodulation, our system achieves a ~100× increase in SRH imaging speed compared to established implementations. This performance closes a critical gap between laboratory SRS microscopy and the requirements of surgical guidance, positioning stimulated Raman histology as a practical tool for intraoperative decision support and high-throughput, slide-free pathology.

Keywords: coherent Raman scattering, stimulated Raman scattering (SRS), stimulated Raman histology, real-time histology

Invited Lectures

[Abstract:0068]

Ultra-Rapid, Quantitative, Label-Free Antibiotic Susceptibility Testing (AST) Via SERS Detected Purine Metabolites: The World's Fastest AST Methodology

Ranjith Premasiri[1], Allen Fraiman[1], Wei Yu[2], Aniket Sharma[3], Bledar Bisha[3], Keith Carron[2], Lawrence Ziegler[1]

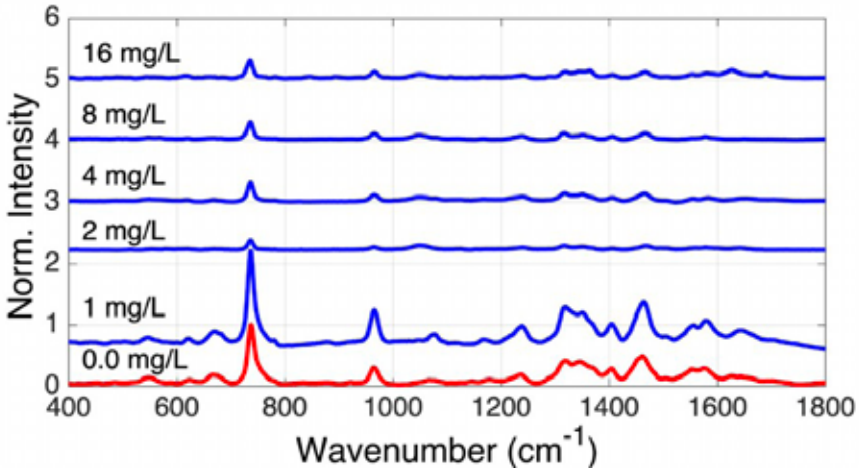
[1]Department of Chemistry & The Photonics Center, Boston University, Boston, USA
[2]SKM Instruments, Laramie, WY, USA
[3]Department of Animal Science. University of Wyoming, Laramie, WY

Infectious diseases remain one of the greatest challenges to global health, and the growing prevalence of infections resulting from drug-resistant bacteria, in particular, are increasingly recognized as a major and growing 21st century public health problem. In order to facilitate the best antimicrobial prescribing practices and to help reduce the increasing global threat of antibiotic resistance, there is an urgent need for the development of truly rapid antibiotic susceptibility testing (AST) platform that can yield results in a 30 minute to 1 hour timeframe for the best management of infectious diseases. Delays in the start of the most effective antibiotic treatment has deleterious health outcomes. For example, every hour delay in the administration of the correct antibiotic in the treatment of suspected blood infection patients increases the risk of mortality by 9%.

We have discovered that a 785 nm surface enhanced Raman spectroscopy (SERS) based phenotypic methodology (Figure 1) results in accurate minimum inhibitory concentration (MIC) determinations in 1 hour for all tested bacterial strain/antibiotic pairs, including a 30-min drug incubation period (Figure 2). This SERS-AST procedure works for both Gram positive and negative species, for both bactericidal and bacteriostatic antibiotics, and for antibiotics with different initial primary targets of antibiotic activity. The molecular level metabolite-based mechanism of this methodology is described. Bacterial SERS spectra are due to secreted purine nucleotide degradation products (principally adenine, guanine, xanthine and hypoxanthine) resulting from the water washing induced, rapid bacterial stringent/starvation response. Due to the no nutrient conditions, (p)ppGpp alarmone is produced which mediates nucleobase formation from unneeded tRNA and rRNA in these starvation conditions. The rewiring of metabolic responses intended to enhance survival due to the secondary metabolic effects of antibiotic exposure during the 30-min incubation period accounts for the observed dose dependent decrease in SERS spectral intensities (Figure 1) which accurately yield the MIC. This is the fastest demonstrated AST method yielding accurate, clinically relevant MICs and resistant/susceptible determinations. Advances in transforming our demonstrated lab benchtop procedure into a commercially viable platform with an initial target of bloodstream infections which can lead to sepsis is described.

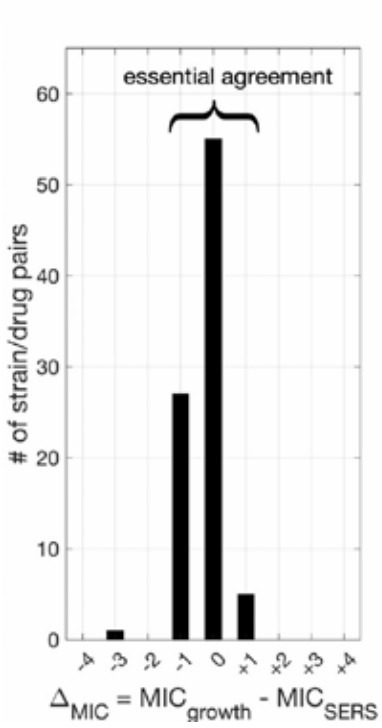
Keywords: SERS, bacteria, antibiotic susceptibility testing, diagnostics, metabolites

Figure 1



SERS intensities of E. faecium 2127 after 30 min incubation with vancomycin.

Figure 2



Summary of essential agreement between growth (24 hr) and SERS-AST (1 hr) determinations of MIC (minimum inhibitory concentration) for ~90 bacterial strain/drug combinations.

Invited Lectures

[Abstract:0083]

Label-Free Detection of Cardiac Amyloid Deposits in Human Tissue by Multiplex CARS Spectroscopic Imaging

Koki Ota[1], Takanori Yamaguchi[2], Toyokazu Otsubo[2], Ryo Suzuki[1], Hideaki Kano[1]

[1]Faculty of Science and Technology, Keio University, Japan
[2]Department of Cardiovascular Medicine, Saga University, Japan

Cardiac amyloidosis is a disorder characterized by the deposition of misfolded proteins, known as amyloid, within cardiac tissue [Yamaguchi et al., J. Am. Heart Assoc. 2022, 11, e024521]. Amyloid is formed when normally folded proteins undergo structural alterations that promote abnormal aggregation. At present, the gold standard for definitive diagnosis is Congo Red staining followed by observation under polarized light microscopy. However, insufficient aggregation can hinder detection by staining, making early diagnosis difficult. Therefore, the development of a reliable method for detecting amyloid deposits is essential for improving patient prognosis.

In this study, we investigated label-free detection of amyloid using a multiplex coherent anti-Stokes Raman scattering (CARS) microscope [Yoneyama et al., APL Photon. 2018, 3, 092408]. A custom-built pulsed laser system with two synchronized outputs was used for the pump beam (1064 nm) and the Stokes beam (supercontinuum) to generate multiplex CARS signals. By comparing two tissue samples, one containing amyloid deposits (Fig. 1, top two panels) and one healthy control (Fig. 1, bottom two panels), we found that the amide I band in amyloid-deposited tissue exhibited a sharper spectral profile. Quantitative evaluation using kurtosis, a statistical measure of spectral sharpness, revealed a clear distinction between amyloid-deposited and healthy tissues.

Keywords: coherent anti-Stokes Raman scattering, CARS, microscopy, human cardiac amyloidosis

Figure 1

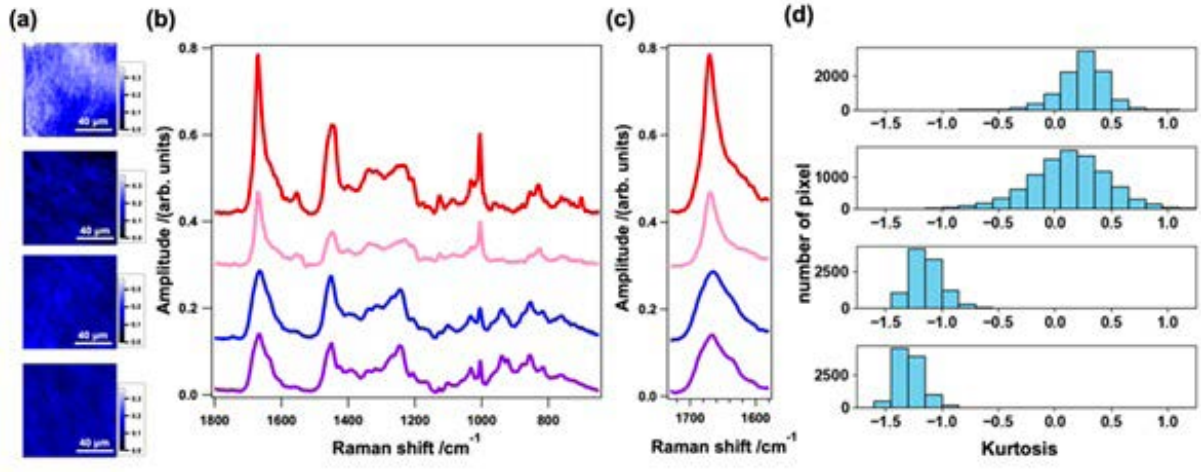


Figure 1. (a) CARS image at the amide I band, (b) Im[\chi^{(3)}] spectra averaged over the image in (a) (the image in (a) and spectra correspond in order from top to bottom), (c) Magnified Im[\chi^{(3)}] spectra in the 1550 cm^{-1} to 1750 cm^{-1} region, (d) Histogram of kurtosis values of the amide I band shown in (c).

Invited Lectures

[Abstract:0224]

Surface-Enhanced Raman Optical Activity of Molecules Using Chirality Induction From Chiral Molecules to Non-Chiral Molecules on A Particle-on-Film Substrate

***Dae Hong Jeong*, Sung Gun Lee**

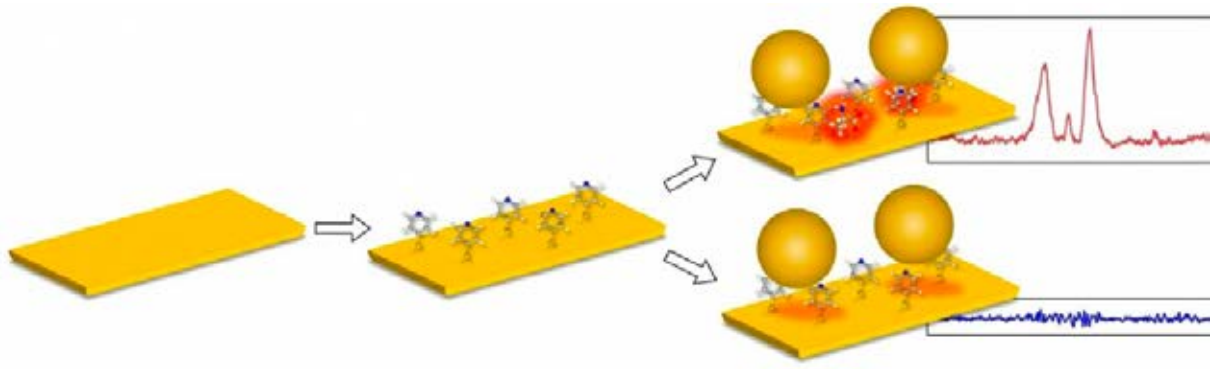
Department of Chemistry Education, Seoul National University, Seoul, Korea

Raman signal difference with LCP and RCP light excitation, known as Raman optical activity (ROA), presents fascinating capabilities as it provides stereo chemical information and so distinguishes chirality of molecules. However, the inherently weak intensity of Raman scattering light has to this point hindered the application of Raman spectroscopy in chiral structures. SERS has been applied to various fields persuing detection of trace molecules owing to its highly sensitive detection capacity caused by localized surface plason enhancement on certain nanostructure of gold and silver metals. Raman optical Surface-enhanced Raman Optical Activity (SEROA) is a promising method for analyzing chiral molecules' molecular chirality and structural changes. However, conventional SEROA measurements face challenges related to substrate stability, signal uniformity, and interference from Electronic Circular Dichroism (ECD).

In this study, we present a uniform and stable substrate for SEROA measurements by utilizing Au nanoparticles on the Au nanofilm structure to confine hotspots to the film-particle junctions and minimize ECD interference. This method also uses the induction of chirality from chiral molecules to non-chiral molecules to overcome the limitation of chiral molecules in SEROA measurement, specifically their lower signal efficiency. Successful chirality transfer is demonstrated through distinguishable SEROA signals when the L/D-Alanine mixture is present. Enantiomeric discrimination of different L/D-Alanine ratios was achieved with linear responses in Circular Intensity Difference (CID). Altogether, the pro-posed chiral-induced SEROA on the AuNP_on_AuNF substrate shows promising potential for detecting and characterizing structural changes in biomolecules, thus making it a valuable tool for various research applications.

Keywords: Surface-Enhanced Raman Scattering, Raman Optical Activity, Nanoparticle on Film, Molecular Chirality

Figure.png



Schematic illustration of the fabrication of AuNP_on_AuNF for measurement of chiral-induced surface-enhanced Ra-man optical activity.

Invited Lectures

[Abstract:0239]

Plasmonic Photothermal Phase Transition of TiO2 Nanoshells Around Gold Nanorods

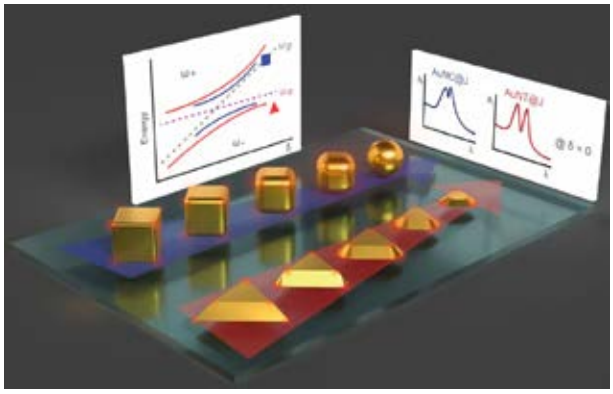
Sangwoon Yoon

Department of Chemistry, Chung-Ang University, Seoul, Korea

Strong plasmon–exciton coupling occurs when a quantum emitter coherently interacts with the confined field of a plasmonic cavity, forming hybrid polariton states. Here, we investigate how nanoparticle curvature affects this strong coupling by assembling gold nanocubes (AuNCs) and nanotriangles (AuNTs) with cyanine dye J-aggregates. Controlled cysteamine etching systematically modifies nanoparticle curvature, enabling direct evaluation of morphology-dependent coupling. Spectral analyses yield vacuum Rabi splittings of 115 meV for AuNCs and 189 meV for AuNTs. As corners round, coupling strength decreases for AuNCs but remains unaffected for AuNTs, mirroring their plasmonic electric field distributions. Comparing coupling strengths with damping rates reveals that AuNCs operate in the intermediate coupling regime due to large plasmon damping, while AuNTs robustly achieve deep strong coupling across all curvatures. Evaluations of mode volume, quality factor, and figure of merit (FOM) further establish AuNTs as superior cavities. While the FOMs for both geometries are relatively insensitive to local curvature, AuNTs consistently exhibit FOMs nearly twice those of AuNCs. These results demonstrate that overall particle shape, rather than corner sharpness, dictates plasmon–exciton strong-coupling efficiency. This study advances the design of plasmonic cavities for enhanced light–matter interactions by identifying key structural and optical parameters.

Keywords: strong coupling, plasmonic cavity, Rabi splitting, J-aggregates, nanoparticle curvature

Plasmon-Exciton Strong Coupling



Systematic etching of gold nanocubes (AuNCs) and nanotriangles (AuNTs) reveals how nanoparticle morphology governs plasmon–exciton strong coupling. While rounding the corners of AuNCs weakens their coupling, triangular geometries robustly preserve deep strong coupling. Quantitative cavity metrics confirm that global geometric architecture, rather than local curvature, dictates the strong-coupling efficiency of hybrid plasmonic platforms.

Invited Lectures

[Abstract:0255]

Raman Spectroscopy for Magnetic Two-Dimensional Materials

Hyeonsik Cheong

Department of Physics and Center for Nano Materials, Sogang University, Seoul, Korea

Two-dimensional (2D) magnetic materials are attracting much interest both for the fundamental understanding of the physics in low dimensions and for possible applications in future spin-based devices. A series of ferromagnetic and antiferromagnetic materials have been identified and many fascinating physical phenomena have been reported [1]. Due to the small volume of atomic-thickness specimens of such materials, optical spectroscopy has been extensively utilize in the study of 2D magnetic materials. Raman spectroscopy, in particular, has been used in the study of 2D antiferromagnetic materials: it has been found that the magnetic ordering often correlates with the changes in the Raman spectrum [2], and low-energy magnons can be detected through low-frequency Raman scattering measurements [3]. More recent studies reveal that the bulk crystal structure may not be conserved in the few-layer limit, and complex domain structures exist. Raman spectroscopic imaging, in combination with electron microscopy provides a detailed picture of such domain structures. In this talk, I will review recent advances in the study of 2D van der Waals magnetic materials using Raman spectroscopy and discuss outstanding issues.

References:

[1] J.-G. Park, et al., Reviews of Modern Physics, in press (https://doi.org/10.1103/2pff-xy6n; arXiv:2505.02355v1).

[2] K. Kim, J.-U. Lee, H. Cheong, Nanotechnology 30, 452001 (2019).

[3] W. Na, et al., ACS Nano 18, 20482 (2024).

Keywords: Raman, Magnetic 2D Materials, Two Dimension, Magnon

Invited Lectures

[Abstract:0258]

Structural Evolutions in the Multiexciton Generation Processes in Slip-Stacked Perylene Dye Array Probed by Time-Resolved Electronic and Vibrational Spectroscopy

Dongho Kim

Department of Chemistry, Yonsei University, Seoul 03722, Korea

Perylene bisimide (PBI) is a quintessential photoactive molecule in various molecular assemblies. Slip-stacked PBI arrays, in particular, exhibit fascinating photophysical phenomena, including excimer formation, charge transfer, and singlet fission. The electronic and structural couplings between adjacent PBI units play a crucial role in exciton localization and delocalization. To investigate the structural dynamics in the excited state, we employed time-resolved vibrational spectroscopy on slip-stacked PBI arrays ranging from dimers to pentamers, shedding light on the formation of localized excited states.

Ground-state Raman spectroscopy reveals key structural features of PBI arrays up to the pentamer. The 110 cm^{-1} mode, corresponding to the intermolecular out-of-plane vibrations of the PBI ring, intensifies progressively from monomer to pentamer without any frequency shift, as supported by TDDFT calculations. Excited-state Raman spectra, obtained via impulsive stimulated Raman spectroscopy (ISRS), reveal low-frequency modes around 100 cm^{-1}, with a slight redshift from dimer to pentamer, indicating weaker coupling in the excited state compared to the ground state. This observation aligns with exciton localization processes seen in time-resolved electronic spectroscopy.

Moreover, a distinct 40 cm^{-1} mode, prominent in PBI trimers and pentamers, is attributed to collective phonon modes involving the vibrational motion of the entire array. These results highlight the intricate interplay between exciton coupling, delocalization, and structural coupling in PBI arrays. Additionally, the fluorescence enhancement observed in longer PBI arrays points to potential applications in optoelectronic devices, such as organic light-emitting diodes.

Keywords: Time-resolved Raman, Time-resolved Electronic, PBI Array, Structural Dynamics, Impulsive Stimulated Raman Spectroscopy

Invited Lectures

[Abstract:0304]

AI-Assisted Plasmonic Nanopores for Single-Molecule SERS Detection of Post-Translational Modifications

Jianan Huang

Research Unit of Health Sciences and Technology (HST), Faculty of Medicine, Research Unit of Disease Networks, Faculty of Biochemistry and Molecular Medicine University of Oulu, Room 372B, Aapistie 5A, 90220 Oulu, Finland

Proteins are the workhorses in biological systems that can be used to characterize cellular functions and progress of diseases as biomarkers. Compared to DNA, proteins are folded 3-dimentional structures and consist of 20 proteogenic amino acids with different charges and hundreds of post-translational modifications (PTMs). Current mass spectrometry method for protein analysis and sequencing needs 1 million molecule copies, which is challenging to detect low-abundance PTMs. The fact that proteins cannot be amplified results in a serious lag of proteomics behind genomics and transcriptomics, hampering not only mechanistic studies but also clinical applications such as early disease diagnosis. These features thus required single-molecule methods for protein PTM analysis. For example, discriminating low-abundance hydroxylation is a crucial and unmet need for early disease diagnostics and therapeutic development due to the small hydroxyl group with 17.01 Da.

In this talk, I will present the recent work in my group in combining plasmonic nanopores [1,2] with artificial intelligence-assisted surface-enhanced Raman spectroscopy (SERS) for single-particle trapping and single-molecule detection. In fact, each amino acid and their PTMs have their own fingerprint Raman scattering signals that can be used for sequencing. But the Raman signals of single amino acids were too weak to be detected. By trapping single gold nanoparticle in a gold nanopore to generate a single plasmonic hot spot in the nanogap, the Particle-in-Pore sensor achieved detecting single-molecule SERS detection of 20 amino acids.[3] By integrating deep learning analysis of convolutional neural network model with the Particle-in-pore sensor, we have demonstrated the first single-molecule SERS detection of small PTMs including hydroxylation[4] and phosphorylation[5] with >95% accuracies. Our works have paved a ground-breaking way to nanopore-enhanced SERS analysis and sequencing of single proteins.

References:

[1] J.A. Huang, et al., Nature Communications 10, 5321 (2019) DOI:10.1038/s41467-019-13242-x

[2] J.A. Huang, et al., Angewandte Chemie International Edition, 59, 11423-11431 (2020), DOI: 10.1002/anie.202000489

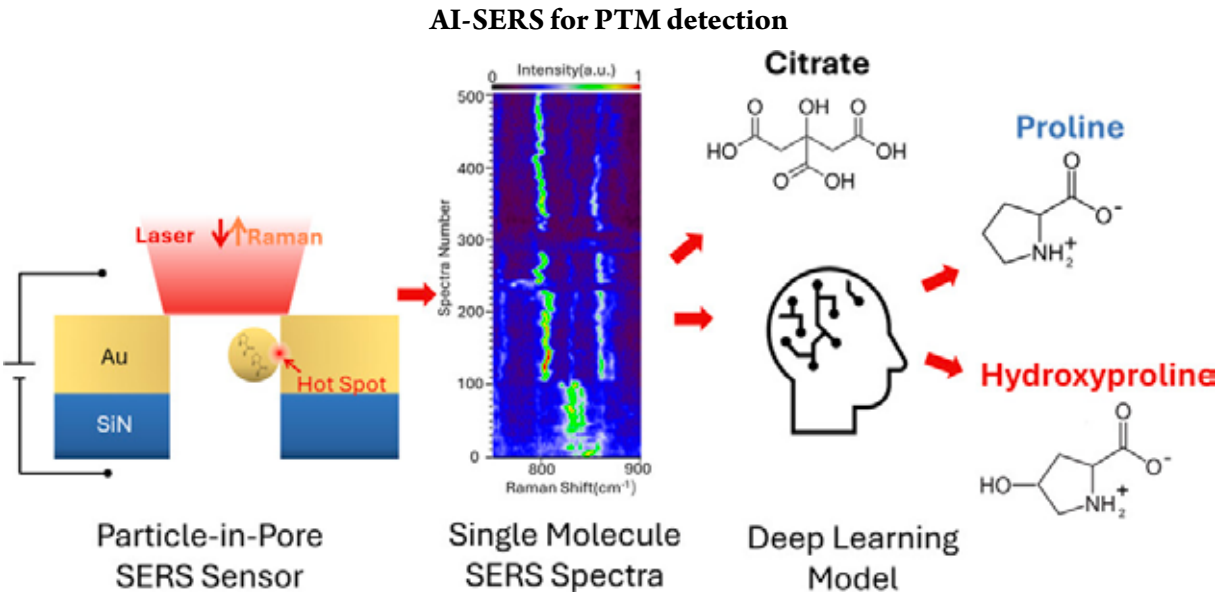
[3] Yingqi Zhao et al., ACS Photonics, 2022, 9 (3), 730-742. DOI: 10.1021/acsphotonics.1c01825

[4] Yingqi Zhao et al., Nano Letters, 2025, 25(18): 7499-7506. DOI: 10.1021/acs.nanolett.5c01177

[5] Mulusew M Yaltaye et al., The Journal of Physical Chemistry Letters, 2025, 16(33): 8418-8426. https://pubs.acs.org/doi/full/10.1021/acs.jpclett.5c01753

Keywords: SERS, nanopore, deep learning, AI, post translational modification, single molecule

Invited Lectures



Schematic of using the plasmonic nanopore for single-molecule SERS detection of PTMs.

Invited Lectures

[Abstract:0313]

Raman Spectroscopy and Microscopy for Accelerated Pharmaceutical Development: Applications From Preclinical to Commercialization

Duohai Pan

Drug Product Development, Bristol Myers Squibb, New Brunswick, NJ 08903, USA

Raman spectroscopy integrated with chemical imaging is a transformative analytical platform with broad and growing applications across the pharmaceutical industry. This presentation highlights its utility — from pre-clinical studies to drug product formulation and process development — illustrating how molecular fingerprints from Raman spectroscopy directly inform critical quality attributes (CQAs) of drug product.

Case studies spanning oral solid-dosage and sterile protein-based drug development are presented: (a) Raman and Terahertz spectroscopy together deliver a rapid, powerful solid-state characterization tool for identifying and distinguishing crystalline API forms, enabling robust polymorph screening and drug substance selection to ensure stability and efficacy from early development through clinical trials. (b) As a sensitive and selective PAT tool, Raman monitors API form conversion, drug–drug and drug–excipient interactions, API agglomeration, and content uniformity in tablet and capsule formulations — while quantifying process- and stability-induced API form changes to control drug product quality and performance. (c) In biotherapeutics, Raman enables comprehensive particulate characterization — discriminating proteinaceous particles, silicone oil droplets, and foreign particles in the critical subvisible range (1–100 μm) — providing mechanistic insight into particulate formation and guiding mitigation strategies in formulation and manufacturing. (d) For emerging modalities such as lipid nanoparticles (LNPs), conventional Raman combined with stimulated Raman scattering (SRS) imaging elucidates structure–function relationships governing drug release mechanisms, ensuring LNPs consistently meet performance targets.

Keywords: Lattice vibrations, polymorphs, formulation, critical quality attribute (CQA), Process Analytical Technology (PAT)

Invited Lectures

[Abstract:0419]

Rapid Coherent-Raman Optical Activity (CARS-ROA) Spectroscopy in the Low Millisecond Regime

Vikas Kumar, Till Reichenauer, Luca V. Supovec, Sebastian Schlücker

Department of Chemistry (Physical Chemistry), Center for Nanointegration Duisburg-Essen (CENIDE) University of Duisburg-Essen, 45141 Essen, Germany

Spontaneous Raman Optical Activity (sROA) is a powerful chiroptical spectroscopic tool for noninvasive identification of chiral molecules based on their molecular vibrational signatures. However, sROA suffers from very weak signals, hence requiring from several tens of minutes up to a few hours for spectral acquisition. This makes it inappropriate for practical uses and deemed unsuitable for analyzing fast processes involving chiral molecules. As early as 1980, Bjarnason et al. [1] theoretically proposed a nonlinear version of sROA called Coherent Anti-Stokes Raman Scattering-Raman Optical Activity (CARS-ROA). The CARS-ROA signal is expected to be ~104 to 105 times stronger than the sROA signal. The first experimental CARS-ROA spectrum was recorded by Hiramatsu et al [2] in 2012, requiring 30 min of acquisition time. Later, in 2015 Hiramatsu et al. [3] using high power visible lasers and in 2023 our group [4] using typical low power broadband CARS lasers squeezed the acquisition time to 1-min for a CAR-ROA spectrum of β-pinene liquid. However, this is still too slow for monitoring kinetics taking place on the millisecond to second scale. Here, we demonstrate our recently developed CARS-ROA spectroscope that can acquire a CARS-ROA spectrum in just 1-ms which is ~60000 times faster than the previously available instruments. Figure 1 shows the example of CARS-ROA spectra acquired by it. In the conference, the details and development of this new CARS-ROA spectroscopy instrument will be presented.

References:

[1] Bjarnason et al. Journal of Chemical Physics 1980, 72 (7)

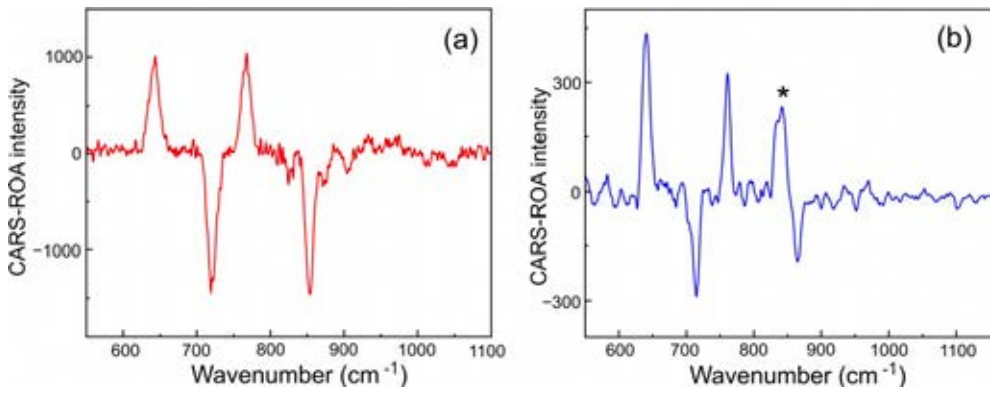
[2] Hiramatsu et al. Physical Review Letters 2012; 109(8):083901

[3] Hiramatsu et al. Optics Letters 2015, 40 (17), 4170-4173

[4] Kumar et al. Journal of Raman Spectroscopy 2023, 54 (9)

Keywords: CARS-ROA, Raman Optical Activity, Vibrational Spectroscopy, Molecular Chirality

Figure 1



(a) CARS-ROA spectrum of neat (-)-β-pinene obtained with 1 ms acquisition time. (b) CARS-ROA spectrum of a 2-vol% solution of (-)-β-pinene in diethyl ether. The * denotes the leakage of a solvent peak.

Invited Lectures

[Abstract:0425]

Chiral-Raman and Its Applications

Jihyeon Yeom

KAIST, Korea Advanced Institute of Science and Englineering

In this talk, I will introduce the fundamental principles of Chiral-Raman spectroscopy and discuss how it can reveal chirality from the molecular to the atomic and mesoscale levels. I will then highlight recent advances in applying incident circular polarization ROA to inorganic nanomaterials, including statistically resolved two-dimensional chirality mapping of chiral selenium films and the identification of handedness in extended material systems. Finally, I will discuss emerging applications of Chiral-Raman platforms in chiroptoelectronics, structural analysis of functional nanomaterials, encryption and information encoding based on polarization-dependent optical responses, and label-free bioanalysis, where chiroptical spectral fingerprints can be combined with data-driven methods for sensing and diagnosis. These examples illustrate how Chiral-Raman spectroscopy is evolving from an analytical technique into a broader materials and biointerface platform for next-generation photonic, electronic, biomedical, and secure information technologies.

Keywords: Chirality, Raman, Chiral Nanomaterials

Invited Lectures

[Abstract:0449]

Bioorthogonal Vibrational Probes Enable Raman Imaging of Enzyme Activity in Cells

***Samir F. El-Mashtoly*[1], *Annaleah Hanske*[2], *Constanze Schultz*[1], *Axel Hentsch*[2], *Senthilvelrajan Kaniyappan*[3], *Rainer E. Martin*[3], *Mario Van Der Stelt*[4], *Christoph Krafft*[1], *Uwe Grether*[3], *Marc Nazare*[2], *Anne T. G. De Paepe*[3], *Jürgen Popp*[1]**

[1]*Leibniz Institute of Photonic Technology, Jena, Germany, Institute of Physical Chemistry, Abbe Center of Photonics, Friedrich-Schiller-University, Jena, Germany*
[2]*Leibniz Forschungsinstitut für Molekulare Pharmakologie, Berlin, Germany*
[3]*Roche Pharma Research & Early Development (pRED), Roche Innovation Center Basel, F. Hoffmann-La Roche Ltd., Basel, Switzerland*
[4]*Leiden Institute of Chemistry (LIC), Universiteit Leiden, CC Leiden, Netherlands*

Elucidating the localization and functional behavior of enzymes involved in lipid metabolism is essential for understanding cellular signaling networks. However, current imaging strategies face limitations: fluorescence-based methods often require large reporter groups that may influence molecular properties, while label-free approaches typically lack molecular selectivity.

Vibrational spectroscopic techniques provide an alternative by enabling chemically specific detection without external fluorophores. In particular, spontaneous Raman and stimulated Raman scattering (SRS) microscopy allow visualization of small molecular tags introduced into biological systems. Nevertheless, selective targeting of individual enzymes using these approaches remains underexplored.

In this study, we develop bioorthogonal probes incorporating an alkyne functionality for the detection of monoacylglycerol lipase (MAGL) in cellular environments. The alkyne group gives rise to a characteristic signal within the cellular Raman-silent spectral region, enabling sensitive and selective detection using both spontaneous Raman and SRS microscopy. Imaging results demonstrate efficient probe internalization and accumulation in intracellular regions associated with lipid metabolism, in agreement with the known biological role of MAGL.

Fast imaging with subcellular resolution is achieved using SRS microscopy. In addition, complementary fluorescence lifetime imaging microscopy (FLIM), employing a structurally related fluorescent probe, verifies target engagement and demonstrates the compatibility of vibrational and fluorescence-based imaging strategies.

To broaden the scope, multiple probe variants were investigated, including covalent inhibitors and activity-dependent turn-on probes. These results underline the flexibility of bioorthogonal vibrational probes for selective visualization and functional investigation of enzymes in complex cellular systems.

Overall, this work demonstrates the potential of Raman-based bioorthogonal probes as minimally invasive tools for studying lipid-associated enzymatic processes with high chemical specificity.

Keywords: Raman microscopy, Bioothogonal probes, Enzyme imaging, Lipid metabolism

Invited Lectures

[Abstract:0453]

From Nanoplasmonics to Surface-Enhanced Spectroscopies: an Atomistic Perspective

Tommaso Giovannini

Department of Physics, University of Rome Tor Vergata, Rome, Italy

The optical response of plasmonic nanostructures can be tuned by varying their shape, size, and chemical composition [1]. Peculiar phenomena arise when a molecular system is adsorbed on the surface of plasmonic materials, ranging from surface-enhanced spectroscopies to photocatalysis [2]. The accurate description of the optical properties of the plasmonic substrates is thus crucial for an understanding of the physical phenomena occurring at the plasmon resonance frequency.

Here, we present an atomistic, yet classical, approach to predict the plasmon properties of nanostructures of complex shapes. The method is general enough to describe any plasmonic material, including noble metal nanoparticles (Ag and Au) [3] and metal alloys [4]. We show that our classical approach for plasmonics can correctly reproduce reference ab initio data [3,5], and experimental trends [3-4], and can be applied to large-scale nanoplasmonic simulations [6]. The method is also coupled to a quantum mechanical (QM) description of the molecular system adsorbed on the nanostructure surface [5]. The resulting mixed QM/classical method is then extended to various spectral signals, from surface-enhanced Raman scattering to surface-enhanced fluorescence.

References:

[1] K. L. Kelly et al., J. Phys. Chem. B 2003, 107, 668.

[2] J. Langer et al. ACS Nano 2019, 14, 28.

[3] T. Giovannini et al., ACS Photonics 2022, 9, 3025.

[4] L. Nicoli et al. Front. Photon. 2023, 1199598.

[5] T. Giovannini et al., Nanoscale, 2019, 11, 6004.

[6] T. Giovannini et al. Nano Lett. 2025, 25, 10802.

[7] P. Lafiosca et al., J. Chem. Theory Comput., 2023, 19, 3616.

Acknowledgments

This work has received funding from the ERC under the European Union's Horizon Europe research and innovation programme (grant no. 101219149, project CHOPIN). Views and opinions expressed are however those of the author only and do not necessarily reflect those of the European Union or ERC Executive Agency. Neither the European Union nor the granting authority can be held responsible for them.

Keywords: SERS, nanoplasmonics, modeling, atomistic, theory, quantum

Invited Lectures

[Abstract:0463]

Application of Raman Imaging to Liquid-Liquid Phase Separation of Proteins: Quantitative Analysis of Coexisting Components

Takakazu Nakabayashi

Graduate School of Pharmaceutical Sciences, Tohoku University, Sendai, Japan

We have investigated liquid–liquid phase separation (LLPS) of biopolymers using Raman imaging [1–6]. In this presentation, we report the identification and quantitative analysis of molecular components within LLPS droplets. LLPS forms biomolecule-rich droplets, and various neurodegeneration-related proteins undergo LLPS followed by a transition into pathogenic aggregates. Although RNA has been proposed to regulate the aggregation process, its precise role remains unclear. Raman imaging enables label-free, quantitative analysis of molecular components within droplets. We also demonstrated that molecular concentrations within droplets can be determined by combining Raman imaging with the water Raman band. Using this approach, we quantified droplets of fused in sarcoma (FUS), a protein implicated in amyotrophic lateral sclerosis (ALS), in the presence of RNA. In a buffer solution, FUS droplets aggregated within one hour in the absence of RNA. In contrast, the addition of short-chain RNAs stabilized the droplets regardless of sequence. Raman bands due to RNA were clearly observed within the droplets, indicating RNA enrichment. Quantitative analysis showed the RNA concentration of 3-6 mM, consistent with charge neutralization, suggesting that electrostatic interactions drive RNA incorporation. This enrichment maintains the liquid state and inhibits aggregation by blocking FUS-FUS direct interactions. In contrast, long-chain RNAs did not accumulate within droplets and instead promoted their dissolution, thereby suppressing aggregation. Furthermore, Raman imaging of living cells revealed that endogenous RNA is selectively enriched within intracellular FUS droplets, providing direct in vivo evidence of RNA enrichment. These results indicate that RNA regulates LLPS of FUS in a length-dependent manner, indicating that RNA inhibits FUS aggregation by incorporating into the droplets.

References:

[1] T. Nakabayashi, et al., J. Phys. Chem. B 129 (2025) 8087 (Review).

[2] K. Murakami, et al., Chem. Sci. 12 (2021) 7411.

[3] K. Yokosawa, et al., J. Phys. Chem. Lett., 13 (2022) 5692.

[4] R. Shibuya, et al., Anal. Chem. 96 (2024) 17078.

[5] T. Ogura, et al., JACS Au 5 (2025) 5749.

[6] M. Machida, et al., JACS Au in press.

Keywords: Liquid-liquid phase separation, Neurodegenerative-related protein, RNA, Living cell, Raman imaging

Invited Lectures

[Abstract:0473]

Advanced Drug Monitoring of Anti-İnfectives Exploiting Deep-UV Raman Spectroscopy and Fiber Sensors

Torsten Frosch

Biophotonics, TU Darmstadt, Darmstadt, Germany

Raman spectroscopy provides a versatile platform for molecularl selective monitoring of antiinfective drugs across scales - ranging from mechanistic drug–target interaction studies to quantitative therapeutic drug monitoring in complex clinical matrices. In this contribution, elaborate optical fiber sensors and and deep-UV Raman approaches are advanced to address complementary analytical challenges: (i) high-throughput spectroscopic analysis of weak drug–target interactions and (ii) highly sensitive detection of antiinfective drugs in body fluids.

The excellent chemical specificity of highly spectrally resolved Raman difference spectroscopy enables detailed analysis of molecular interactions between antimalarial drugs and heme-derived target structures involved in malaria pigment formation. Weak biomolecular interactions, such as π–π stacking and hydrogen bonding, typically induce only minor perturbations of molecular force constants and correspondingly small shifts in the Raman spectra. To resolve these effects, parallelized Raman difference spectroscopy was employed to investigate interactions between chloroquine and hematin with enhanced spectral resolution [Anal Chem, 2024, 96(8):3345–3353]. Resonance Raman excitation combined with two-dimensional correlation spectroscopy, density functional theory (DFT) calculations, and normal coordinate structural decomposition analysis was further applied to characterize artesunate interactions with β-hematin. Stepwise variation of drug molar ratios revealed systematic changes in porphyrin vibrational modes, enabling identification of mono- and di-meso-alkylated complexes and providing molecular insight into drug-induced perturbations of hemozoin formation [Anal Chem, 2023, 95(34):12719-12731].

Complementary advances in fiber-enhanced Raman spectroscopy and deep-UV excitation significantly improve signal generation and collection efficiency, enabling label-free quantification of antiinfective drugs in urine and plasma at clinical concentrations, with detection limits in the single-digit μM or $mg{\cdot}mL^{-1}$ range [Nature Communications Medicine, 2025. 5(1); Clinical Spectroscopy, 2023, 5, 100026]. Systematic evaluation further demonstrates the influence of biological reference matrices and sample preparation on quantitative accuracy [Nature Communications Medicine, 2025. 5(1)].

Together, these results highlight the capability of advanced Raman methodologies for high-throughput analysis of drug–target interactions and sensitive, matrix-tolerant therapeutic drug monitoring, underscoring the expanding role of vibrational spectroscopy in antiinfective research and translational biophotonics.

Acknowledgment: Funding by the Hessian research funding program LOEWE/2/18/519/03/11.001(0011)/126 is highly acknowledged.

Keywords: therapeutic drug monitoring (TDM), Fiber-enhanced Raman spectroscopy (FERS), DUV-Raman drug sensing, drug-target interaction analysis, antiinfectives

Invited Lectures

[Abstract:0535]

Regulation Mechanisms of SERS Activity in Organic Semiconductor Composites

***Shuang Guo*[1], *Hye Jin Chang*[2], *Lei Chen*[3], *Young Mee Jung*[2]**

[1]*Key Laboratory of Preparation and Applications of Environmental Friendly Materials, Ministry of Education, College of Chemistry, Jilin Normal University, Changchun 130103, China*
[2]*Department of Chemistry, Institute for Molecular Science and Fusion Technology, Kangwon National University, Chuncheon 24341, Republic of Korea*
[3]*School of Materials Science and Engineering, Jilin Jianzhu University, Changchun 130118, China*

Organic semiconductors have emerged as promising SERS-active substrates because of their tunable electronic structures, adjustable molecular orbitals, good molecular compatibility, and potential for regulating interfacial charge transfer beyond conventional electromagnetic enhancement. In this work, we focus on how electronic-structure modulation in organic and carbon-based semiconductor materials governs charge transfer processes and SERS activity. First, PEDOT:PSS is used as a representative π-conjugated organic semiconductor to investigate the influence of molecular orbital delocalization on SERS enhancement. Temperature-mediated resonance structure transitions of PEDOT regulate the delocalization of molecular orbitals, thereby strengthening substrate–probe electronic coupling and promoting interfacial charge transfer, as supported by absorption spectroscopy and density functional theory calculations. Furthermore, we extend this concept to graphene quantum dots with distinct topological edge structures, namely armchair and zigzag edges, to explore how edge-dependent electronic states affect SERS activity and charge transfer capability. We aim to clarify the relationship between orbital delocalization, edge-state electronic structure, and charge transfer efficiency in semiconductor-based SERS systems. These studies provide new insights into the chemical enhancement mechanism of SERS and offer a rational strategy for designing highly sensitive organic semiconductor composite SERS substrates. Detailed results will be presented at the conference.

Keywords: SERS, organic Semiconductor, charge transfer, PEDOT:PSS, armchair and zigzag edges

Invited Lectures

[Abstract:0562]

AI-Assisted Surface-Enhanced Raman Spectroscopy from Spectral Fingerprints to Diagnosis

***Omer Aydin*[1], *Münevver Akdeniz*[1], *Zakarya Al-shaebi*[1], *Pınar Sağıroğlu*[2], *Mustafa Altay Atalay*[2], *Serra Ilayda Yerlitas Taştan*[3], *Gözde Ertürk Zararsız*[3], *Gokmen Zararsiz*[3], *Muzaffer Keklik*[4], *Alısan Kayabolen*[5]**

[1]*Department of Biomedical Engineering, Erciyes University, Kayseri, Türkiye*
[2]*Department of Medical Microbiology, Erciyes University, Kayseri, Türkiye*
[3]*Department of Biostatistics, Erciyes University, Kayseri, Türkiye*
[4]*Department of Hematology, Erciyes University, Kayseri, Türkiye*
[5]*Department of Medical Biology, Koc University, Istanbul, Türkiye*

Surface-enhanced Raman Spectroscopy (SERS) has attracted growing attention in medicine because of its strong potential for molecular fingerprinting, biomarker discovery, and disease diagnosis. Although substantial progress has been achieved in the physical, material, and nanostructural design of Raman-active and SERS platforms, the routine clinical implementation of these technologies remains limited. This gap is driven not only by challenges in reproducibility and spectral variability, but also by the difficulty of extracting robust and clinically meaningful information from highly complex biological datasets. Therefore, advancing Raman-based diagnostics requires not only improved sensing platforms but also application-oriented studies focused on direct analysis of real biological and clinical samples.

In this context, artificial intelligence (AI)-assisted SERS has emerged as a powerful strategy to overcome current translational barriers and move spectral technologies closer to clinical practice. By enabling advanced interpretation of large, heterogeneous, and information-rich spectral datasets, AI can improve classification performance, reduce the impact of noise and variability, and reveal subtle biochemical signatures associated with disease states. In this talk, we will present our AI-assisted SERS studies across diverse biologically and clinically relevant applications, including the detection of antimicrobial resistance-related profiles, the discrimination of cancer directly from serum samples, the classification of bacteria-associated infection signatures in serum, and the analysis of virus-like particles and extracellular vesicles. Our findings demonstrate that the integration of AI with SERS provides a robust framework for multiclass classification and clinically relevant spectral interpretation, highlighting its promise for disease diagnosis, liquid biopsy, and infection monitoring. Overall, this approach represents an important step toward transforming spectral fingerprints into actionable diagnostic insight.

This work has been partially supported by the Erciyes University Scientific Research Projects Coordination Unit (BAP) under grant number: FBAÜ-2023-12265.

Keywords: Surface-enhanced Raman spectroscopy, artificial intelligence, diagnosis, exosome, virus like particles, antimicrobial resistance

Invited Lectures

[Abstract:0564]

Raman Spectroscopy Techniques for Intra-Operative Diagnosis in Cancer Surgery

***Radu Boitor*, Ioan Notingher**

School of Physics and Astronomy, University of Nottingham, Nottingham, United Kingdom

Raman spectroscopy is a powerful technique for analysing biological tissue at a microscopic level. The talk focuses on molecular imaging of tissue for fast detection of positive margins during cancer surgery. Selective sampling approaches that combine auto-fluorescence imaging, optical coherence tomography and Raman spectroscopy exploit the speed and molecular specificity of these techniques to allow accurate detection of positive margins within timescales compatible with intra-operative clinical use. The presentation will show the latest results on clinical integration and validation of the technique for skin and breast cancer surgery, focusing on diagnostic test accuracy studies. The presentation will also highlight the potential of this technology for broader applications in surgical margins and in-vivo diagnosis for to other cancer types.

Keywords: Raman Spectroscopy, Cancer Detection, Surgical Margins, Optical Coherence Tomography

Invited Lectures

[Abstract:0578]

Visualization of In-Situ Marine Biodegradation İn Poly(3-Hydroxybutyrate) Using Three-Dimensional Raman Mapping

Harumi Sato

Graduate School of Human Development and Environment, Kobe University, 3-11 Tsurukabuto Nada-ku, Kobe 657-8501, Japan

Recently, low-frequency spectroscopy has attracted much attention in the fields of biomolecules, medicine, and polymer materials. In particular, Raman spectra in the low-frequency region are highly sensitive to the higher-order structure, crystalline structure, lattice expansion, and intermolecular interactions in polymers, making this technique a powerful tool for evaluating various material properties, inter- and intramolecular interactions including hydrogen bonding.

Meanwhile, microplastics, which are generated through the fragmentation of plastic waste released into the marine environment, have become a serious environmental issue. Addressing this problem requires both elucidation of the mechanisms of biodegradation in marine environments and the replacement of conventional plastics with biodegradable alternatives. Therefore, in this study, poly(3-hydroxybutyrate) (P(3HB)) and its copolymers, which are biodegradable plastics, were investigated. Low-frequency Raman spectroscopy was employed to evaluate structural changes and variations in intermolecular interactions during the marine degradation process, with the aim of elucidating the mechanism of marine biodegradation.

As a result, it was confirmed that marine degradation of P(3HB) preferentially occurred in the amorphous regions of the film surface, which were subsequently released into seawater. Consequently, the crystallinity of the polymer film surface increased with the progression of marine degradation. Moreover, these structural changes were successfully visualized.

Keywords: Raman imaging, low-frequency, Marine biodegradation, Poly(3-hydroxybutyrate)

Invited Lectures

[Abstract:0581]

Unravelling Catalytic Reaction Mechanisms with In Situ Tip-Enhanced Raman Spectroscopy

Naresh Kumar

ETH Zurich, Switzerland

Mechanistic understanding of heterogeneous catalytic reactions remains challenging because key elementary steps often occur at nanoscale active sites and on short time scales that are averaged out in conventional spectroscopic measurements. Tip-Enhanced Raman Spectroscopy (TERS), which combines the spatial precision of scanning probe microscopy with the chemical sensitivity of Raman spectroscopy, provides a powerful approach to probe surface chemical transformations beyond the diffraction limit and under working conditions [1–3].

In the first part of this talk, I will demonstrate how STM-based in situ TERS, combined with density functional theory (DFT) modeling, can provide real-time mechanistic insights into catalytic nitroarene hydrogenation on a well-defined Pt(111) surface [4]. Using a close-packed monolayer of chloronitrothiophenol (CNTP) on atomically flat Pt(111), we monitored the hydrogenation reaction at a single plasmonic junction under ambient H_2 exposure. Time-sequenced TERS spectra captured the dynamic conversion of CNTP to chloroaminothiophenol (CATP), revealed by the disappearance of the NO_2 stretching mode and characteristic shifts in the C–S and C=C vibrational bands. The reaction proceeded with a characteristic time scale of approximately 6 s, demonstrating the capability of in situ TERS to follow catalytic transformations in real time at the nanoscale.

In the second part of the talk, I will discuss how first-principles DFT calculations were used to interpret the experimentally observed dynamics and establish a molecular-level reaction mechanism. The calculations show that CNTP desorption from Pt(111) occurs rapidly, while bending of CNTP toward the surface is barrierless and exergonic at reduced surface coverage. The first hydrogen addition to the nitro group is facile, whereas the second hydrogen addition is kinetically most demanding and matches the experimentally observed time scale, identifying it as the rate-determining step.

Overall, this work highlights how in situ TERS integrated with DFT modeling can bridge nanospectroscopy, surface science, and theory to unravel catalytic reaction mechanisms on nonplasmonic metal catalysts.

Invited Lectures

[Abstract:0600]

Stimulated Raman Scattering Microscopy for Cellular Analysis And Semiconductor Characterization

***Yasuyuki Ozeki*[1,2]**

[1]*Research Center for Advanced Science and Technology, The University of Tokyo, Tokyo, Japan*
[2]*Department of Electrical Engineering and Information Systems, The University of Tokyo, Tokyo, Japan*

Stimulated Raman scattering (SRS) microscopy provides vibrational contrast with much faster acquisition than spontaneous Raman microscopy. This combination of chemical selectivity and speed makes the same nonlinear imaging framework applicable to dynamic biological observations and spatially resolved materials characterization. This presentation describes recent developments that broaden both the measurement capabilities and application range of SRS microscopy.

For cellular studies, we developed a combined SRS and fluorescence microscope using a rapidly wavelength-tunable source produced by spectral filtering of Yb-fiber-laser pulses and synchronized with a picosecond Ti:sapphire laser. The Raman shift and fluorescence detection channel can each be changed between successive frames, allowing video-rate acquisition of multiplexed vibrational and fluorescence data. Combined with recently developed Raman probes, the SRS microscope enables highly multiplexed imaging, simultaneous sensing of several enzyme activities, and super-resolution SRS imaging. These functions provide complementary molecular and structural views of dynamic interactions among intracellular compartments.

The high sensitivity of SRS is also advantageous for characterizing semiconductors and two-dimensional materials. For example, SRS enables high-resolution imaging of monolayer and few-layer hexagonal boron nitride, a representative two-dimensional material. Its high signal-to-noise ratio also permits lattice-frequency shifts on the order of 0.01 cm^{-1} to be detected, enabling three-dimensional mapping of strain around threading dislocations in wide-bandgap semiconductors and identification of their Burgers vectors. At telecommunication wavelengths, SRS microscopy further enables volumetric measurements inside silicon and GaAs. The resulting Raman-shift maps provide spatially resolved information on strain and temperature, offering a nondestructive approach to semiconductor process evaluation.

Together, these results demonstrate how tunable light sources, multimodal detection, and wavelength selection can adapt SRS microscopy to problems ranging from cellular imaging to volumetric semiconductor metrology.

Keywords: stimulated Raman scattering microscopy, multimodal imaging, Raman probes, semiconductor characterization, strain mapping

ORAL ABSTRACTS

[Abstract:0005] [SERS/TERS/Plasmonics]

Single-Molecule Monitoring of Nucleic Acid Dynamics Using Raman Correlation Spectroscopy in Plasmonic Nanowells

***Peilin Xin*[1], *Yingqi Zhao*[1], *Yuge Liang*[1], *Mulusew W Yaltage*[2], *Aliaksandar Hubarevich*[4], *Viktorija Pankratova*[3], *Shubo Wang*[3], *Jianan Huang*[1]**

[1]*Research Unit of Health Sciences and Technology, Faculty of Medicine, University of Oulu, Oulu, Finland*
[2]*Research Unit of Disease Networks, Faculty of Biochemistry and Molecular Medicine and Biocenter Oulu, University of Oulu, Oulu, Finland*
[3]*Nano and Molecular Systems Research Unit, Faculty of Science, University of Oulu, Oulu, Finland*
[4]*Istituto Italiano di Tecnologia, Genova, Italy*

Label-free monitoring of single molecules by single-molecule surface enhanced Raman spectroscopy (SM-SERS) in plasmonic nanopores can track the molecular dynamics and gain insight into its internal mechanism for applications including catalysis and sequencing. However, challenges including unstable plasmonic hotspot, fast molecule movement, and citrate interference hinder the SM-SERS data analysis and biomedical applications. In this study, we report a new SM-SERS method by sticking a single gold nanoparticle in a gold nanowell in air to generate a fixed plasmonic gap-mode hot spot on the particle surface for continuous single-molecule readout and long-term monitoring of DNA diffusion. The unlimited resident time of the DNA in the hot spot revealed unidirectional and back-and-forth diffusion patterns of different DNAs at single base resolution depending on their sequences as well as cooccupation of the hot spot by

citrate and DNA. Significantly, the spatial resolution of the hot spot was found to be able to cover 2 neighboring nucleobases, 1sugar–phosphate backbone in the DNA, and1 citrate. By using Raman correlation spectroscopy, the diffusion times of nucleobases in the DNAs were calculated as 5–22s depending on molecular structures, while those of citrate were0.1–7 s. Our results were so promising for monitoring biomolecular dynamics that they could be used to investigate oligonucleotide hybridization kinetics and may set the basis for developing SM-SERS sequencing technologies.

Keywords: single-molecule monitoring, SERS, plasmonic hot spot, Raman correlation spectroscopy, citrate interference

[Abstract:0008] [Novel Approaches]

Multimodal Nanoscale Materials Characterization Via Correlative Nano-IR, Raman Microscopy, and Atomic Force Microscopy

Bogdan Sava*, *Amarie Sergiu*, *Andreas Huber

AttocubeSystems GmbH

IRa-SCOPE system represents a new class of correlative nanoscale analytics instrumentation, enabling comprehensive vibrational and mechanical characterization of materials across multiple length scales within a single platform. For the first time, nano-infrared (nano-IR) imaging and spectroscopy are fully integrated with confocal Raman micro-spectroscopy and high-quality Atomic Force Microscopy (AFM). By combining light-based nano-FTIR with force-based tapping AFM-IR, the system ensures optimal sensitivity, spatial resolution, and chemical specificity tailored to diverse sample types.

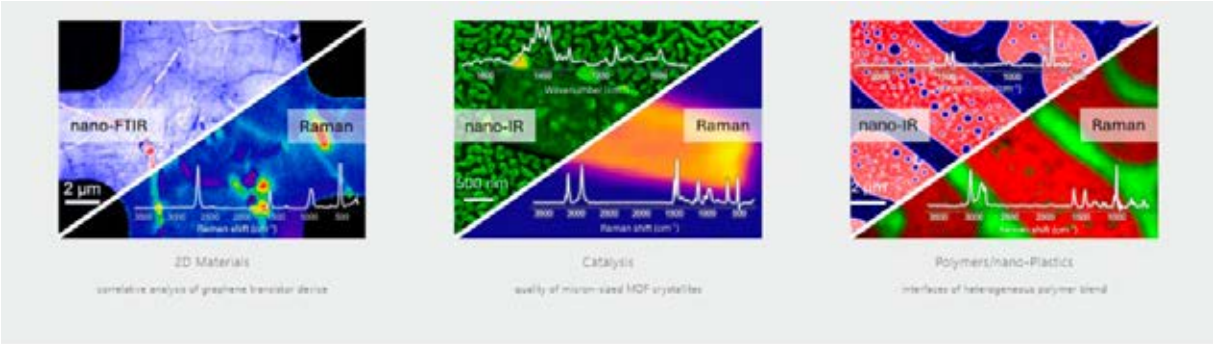
The integration of confocal Raman spectroscopy significantly extends analytical capabilities by providing complementary molecular information and improving chemical identification and validation. In addition, micro-IR spectroscopy based on Laser Direct Infrared (LDIR) reflection-absorption enables rapid, non-destructive sample pre-characterization and efficient identification of regions of interest, all within the same instrument. This correlative workflow minimizes sample handling while maximizing data reliability.

High-performance AFM delivers precise nanoscale topography and mechanical property mapping, supporting quantitative analysis of complex and heterogeneous materials. Advanced sample navigation, intelligent automation, and integrated data management streamline experiments and ensure reproducible, benchmark-level performance.

Leveraging core nanoscale analytics technologies—such as precision nanopositioning, scanning probe microscopy, and correlative optical–probe integration—the IRa-SCOPE is well suited for applications in polymers, nanocomposites, semiconductors, life sciences, and advanced functional materials. The platform sets a new standard for multimodal nanoscale characterization by unifying structural, chemical, and mechanical insights with exceptional data quality and ease of use.

Keywords: correlative microscopy, spectroscopy, material characterization

Correlative Raman & nano-IR Spectroscopy



seamless integration of measurement modes enables comprehensive nano-analysis

[Abstract:0009] [Coherent Raman Imaging]

Fast and Low-Power Super-Resolution Vibrational Imaging Enabled by an Improved Photoswitchable Raman Probe

***Yang Ma*[1], *Satoshi Matsumoto*[2], *Shunsuke Fukuta*[2], *Xiao Wu*[1], *Kazuhiro Kuruma*[3], *Hiroyoshi Fujioka*[3], *Mako Kamiya*[3], *Yasuyuki Ozeki*[3]**

[1]*Department of Electrical Engineering and Information Systems, The University of Tokyo,Tokyo, Japan*
[2]*Research Center for Advanced Science and Technology, The University of Tokyo, Tokyo Japan*
[3]*Department of Life Science and Technology, Institute of Science Tokyo, Yokohama, Japan*

Visualizing diverse subcellular structures with high spatial resolution is fundamental to understanding biological processes and disease mechanisms. Stimulated Raman scattering (SRS) microscopy offers chemically specific imaging with intrinsically narrow spectral linewidths, making it a promising platform for highly multiplexed super-resolution biological imaging. Raman probes, which are molecules engineered with spectrally distinct vibrational signatures, can be targeted to specific cellular structures, and their combination with SRS microscopy enables highly multiplexed imaging across multiple channels. While several strategies have been proposed to break the diffraction limit in SRS imaging, many suffer from limitations such as the need for cell fixation, high power loading, or complicated detection schemes. In addition, realizing multiplexed super-resolution SRS requires sequential acquisition across multiple spectral channels, demanding both fast imaging and photostable probes. Slow acquisition and high optical power accelerate photobleaching of Raman probes, posing a critical barrier to such measurements.

Previously, we developed reversible saturable optical Raman transitions (RESORT) microscopy, a sub-diffraction SRS approach that harnesses reversible photoswitching of a Raman probe to introduce saturation-based nonlinearity into SRS detection. Here, by employing an improved photoswitchable Raman probe derived from our previous design, together with systematic refinements to the optical system, we substantially advance RESORT microscopy for live-cell imaging. Single-pixel dwell time is reduced from 227 μs to 24 μs (~10× faster), and the optical power for probe activation and deactivation is lowered by a factor of 3–4. Spatial resolution is improved from 320 nm (diffraction-limited SRS) to 150 nm by RESORT, representing a greater than 2-fold improvement, as rigorously confirmed by Fourier ring correlation (FRC) analysis, which provides a more reliable estimate than the deconvolution-based approach used in our previous work. Using this improved system, we demonstrate super-resolution SRS imaging of lipid droplets and mitochondria in living mammalian cells. Together, these advances substantially lower the technical barriers to multiplexed super-resolution SRS imaging of living systems.

Keywords: SRS, Super-resolution,Fast imaging

[Abstract:0013] [Biology/Biomedicine]

LabelFree Raman Spectroscopy for Discriminating Breast Cancer Cell Lines and Macrophage Polarization States

***István Csarnovics*[1], *Péter Tóth*[2], *Endre Kokai*[2], *László Virág*[2], *Tamás Váczi*[3], *Gergely Kocsis*[4], *Miklos Veres*[3]**

[1]*Department of Experimental Physics, Institute of Physics, Faculty of Science and Technology, University of Debrecen, Debrecen, Hungary*
[2]*Department of Medical Chemistry, Faculty of Medicine, University of Debrecen, Debrecen, Hungary*
[3]*Institute for Solid State Physics and Optics, HUN-REN Wigner Research Center for Physics, Budapest, Hungary*
[4]*Department of IT Systems and Networks, Faculty of Informatics, University of Debrecen, Debrecen, Hungary*

Raman spectroscopy is a labelfree vibrational spectroscopic technique that provides detailed biochemical information based on the intrinsic molecular fingerprints of biological samples. Its nondestructive nature, minimal sample preparation requirements, and sensitivity to molecular composition make Raman spectroscopy a powerful tool for biomedical cell analysis, particularly in cancer and immunological research. Despite the inherently weak Raman signal, advances in instrumentation and imaging approaches have significantly improved its applicability to cellular studies.

In this work, we demonstrate the use of Raman spectroscopy for discriminating between different breast cancer cell lines and macrophage polarization states, highlighting both methodological aspects and biomedical relevance. Two HER2positive breast cancer cell lines, SKBR3 and JIMT1, were investigated as model systems exhibiting distinct metabolic activities, lipid compositions, and therapeutic response characteristics. Comparative Raman spectral analysis reveals clear differences in key vibrational bands associated with proteins, lipids, and nucleic acids. In particular, variations in the relative intensity and spatial distribution of C–H stretching modes reflect differences in cellular lipid metabolism and membrane organization, enabling reliable differentiation of the two cancer cell lines at the singlecell level. Preliminary results obtained using stimulated Raman scattering (SRS) imaging are also presented, illustrating its potential for highspeed visualization of lipid and protein distributions and for tracking dynamic cellular responses.

The influence of curing agents or therapeutic treatments on SKBR3 and JIMT1 cells was further assessed using Raman spectroscopy, revealing treatmentinduced biochemical changes without the need for fluorescent or chemical labels.

In addition to cancer cells, macrophages representing different functional polarization states—M0 (nonactivated), M1 (proinflammatory), and M2 (antiinflammatory)—were analyzed. Raman spectra of these macrophage phenotypes exhibit distinct biochemical signatures related to changes in lipid content, protein conformation, and intracellular remodeling associated with immune activation and polarization. These spectral differences demonstrate the capability of Raman spectroscopy to monitor immunometabolic alterations in a labelfree manner.

Overall, this study demonstrates that labelfree Raman spectroscopy enables effective discrimination of breast cancer cell lines and macrophage polarization states, providing valuable insights into cellular biochemistry and treatmentinduced changes. These findings highlight the potential of Ramanbased techniques as versatile tools for advanced biomedical research and future diagnostic applications.

Keywords: Labelfree Raman spectroscopy, Breast cancer cell lines, Macrophage polarization, Cancer cell discrimination, Cellular biochemistry, Stimulated Raman scattering (SRS)

[Abstract:0015] [SERS/TERS/Plasmonics]

Integrating Machine Learning with SERS Optophysiology ForEnhanced Neurotransmitter Sensing

***Saba Bashir*, Jean Francois Masson, Malama Chisanga**

Department of Chemistry, University of Montreal, Canada

Real-time monitoring of neurotransmitters in living brain tissue is essential for understanding neuronal communication and the progression of neurological disorders such as Parkinson's disease. Chemical gradients within the extracellular environment surrounding neurons regulate many physiological processes, and disturbances in these gradients can significantly affect neural function. Conventional analytical techniques, including fluorescence microscopy and electrochemical sensing, have provided valuable insights into neurotransmitter activity; however, these methods are limited in their ability to simultaneously detect multiple molecules and capture the full complexity of dynamic neural environments.

Surface-enhanced Raman scattering (SERS) optophysiology combined with optogenetics offers a promising strategy for label-free chemical sensing while enabling optical control of neuronal activity. SERS enhances Raman signals through plasmonic nanostructures, allowing the detection of molecular vibrations and low concentrations of neurotransmitters directly within biological samples. In this work, we extend SERS-based sensing into the short-wave infrared (SWIR) region to improve performance in biological tissues. SWIR excitation allows deeper tissue penetration, reduces background fluorescence, and minimizes photodamage, making it well suited for in vivo applications.

To further enhance signal interpretation, machine learning algorithms will be incorporated to analyze complex Raman spectral data and improve the identification of neurotransmitter signatures. This integrated SWIR-SERS platform will be applied to live mouse brain models to study neurotransmitter release and chemical signaling, providing new insights into neurochemical processes and neurodegenerative disease mechanisms.

Keywords: Surface-enhanced Raman scattering, Optophysiology, Optogenetics, Plasmonic Nanostructures, Neurochemical Sensing

[Abstract:0017] [Novel Approaches]

A New Raman Spectroscopic Approach to Gaseous Tritium Analysis in the Fusion Fuel Cycle Using Hollow-Core Microstructured Optical Fibres

***Jessica Gabb*[1], Rhea Sam[1], William Brooks[1], Michael Wharton[2], Natalie Wheeler[3], Thomas Kelly[3], Hans Christian Mulvad[3], Ian Davidson[3], Peter Horak[3], Joseph Large[2], Simon Steel[2], Anna Denman[2]**

[1]*IS-Instruments Ltd.*
[2]*Amentum*
[3]*University of Southampton*

Reliable gas analysis technologies for the quantification of hydrogen isotopologues, including tritium, are an essential requirement for the fusion industry. This abstract describes the development of a gas phase Raman Spectrometer with high specificity, sensitivity and dynamic range, that utilises a state-of-the-art Hollow Core Microstructured Optical Fibre (HCF). The HCF acts as the instrument probe, the fibre core is filled with the sample gas enabling an extended interaction pathlength between it and the excitation laser which is also guided through the fibre's core. The use of the HCF gives significantly improved sensitivity when compared to other gas sensing Raman instruments.

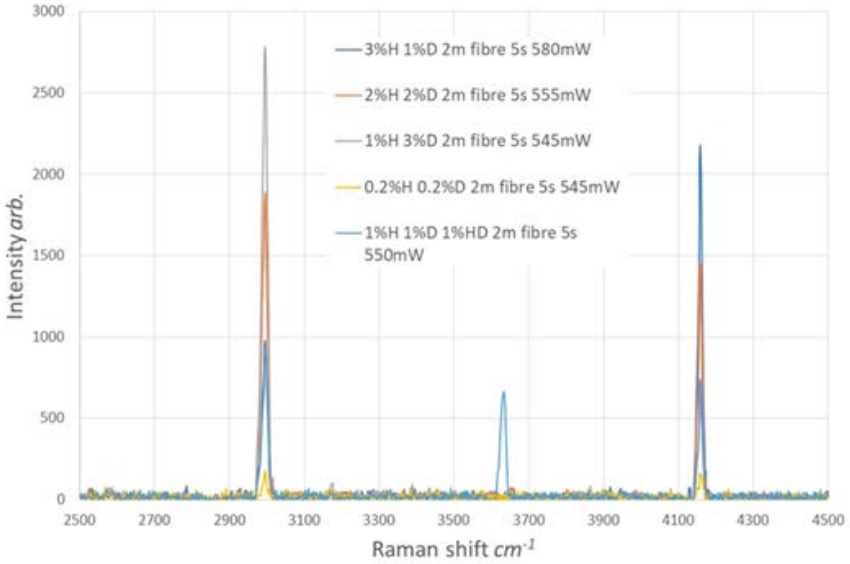
IS-Instruments, ORC and Amentum are focussing on moving this technology beyond a laboratory tool to a deployable on-line instrument for the fusion industry. The initial development focussed on the quantification of gas species of interest to the nuclear industry, from simple diatomic gases e.g. H_2 to heteronuclear organic species. Results showed both a linearity of response across a wide concentration range (ppm-%level) and the potential for low limits of detection (<1ppm H_2). This phase proved that multiple gas species can be measured instantly, simultaneously and non-destructively offering significant advantages over popular technologies such as gas-chromatography.

This benefits the fusion industry, where the rapid on-line measurement of hydrogen isotopologues is essential for the operation of future fusion reactors and the fuel cycle's tritium inventory. The latest developmental work is being carried out under the Fusion Industry Programme and is focussed on the instrument's ability to measure tritium and other hydrogen isotopologues simultaneously, with repeatability and accuracy.

The instrument is currently in place at Amentum's UK tritium facility, with the first successful tritium detection being achieved in March 2025. Results showed identification of all hydrogen isotopologues with a linear response that enables rapid quantification. The spectra showed that all hydrogen species can be characterised in a single measurement time of a few 10s of seconds. Quantification and stability tests demonstrated the instrument's potential as a plant-deployable technology. Additional funding has been granted to extend the testing and to build an updated design ensuring the tritium compatibility of all wetted components.

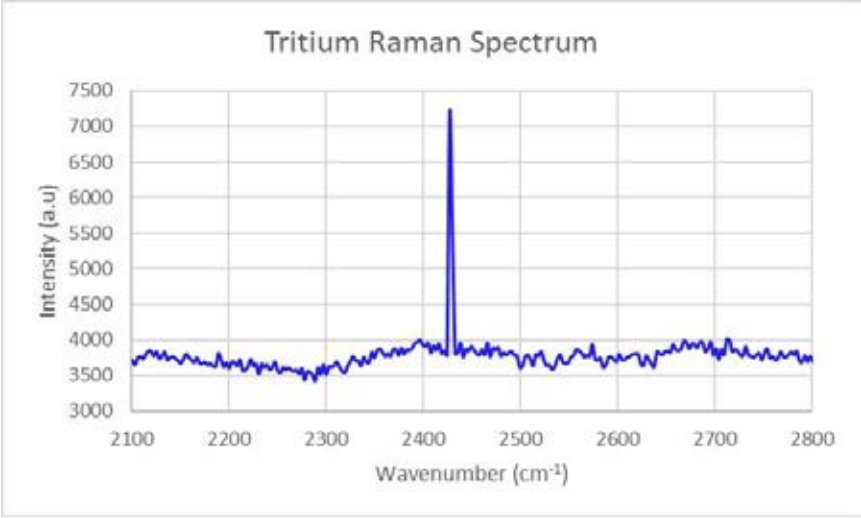
Keywords: Gas, innovation, Hollow-core fibres, fusion.

Raman spectra: H2, D2 & HD at varied concentrations.



The results show the linear Raman response obtained using the instrument to detect the inactive hydrogen isotopologues.

Raman spectrum: The first tritium detection



Results showing the first tritium detection using ISI's instrument. The next phase of testing has begun, therefore a more polished result will be shared at the event.

[Abstract:0019] [SERS/TERS/Plasmonics]

In Situ Raman Reveals CO_2 Assisted Reconstruction of Copper Coordination Polymers Promoting C–C Coupling During CO_2 Electroreduction

***Zeyu Zhang*[1], *Hua Zhang*[1], *Jian Feng Li*[2]**

[1]*College of Materials, Xiamen University, Xiamen, China*
[2]*College of Chemistry and Chemical Engineering, Xiamen University, Xiamen, China*

Electrochemical CO_2 reduction reaction (CO_2RR) is anticipated because of the utilization of clean energy to convert CO_2 into high-value-added chemicals (e.g. CH_4, HCOOH, C_2H_4), but the modification and decoration of catalysts are required to enhance the selectivity and efficiency. Copper coordination polymers (CuCPs) represent an effective strategy for promoting C_2+ products for the ability to activate CO_2[1] and regulate the water dissociation during the reaction[2]. However, due to the participation of organic ligands in the catalytic reaction and the complexity of CO_2RR (e.g., numerous reaction intermediates), conventional characterization is difficult to monitor the evolution of molecular and the CO_2 reduction process.

This study intends to employ in situ surface-enhanced Raman spectroscopy (SERS) combined with isotope substitution analysis to investigate whether molecular ligands participate in the reaction and the in situ evolution of CuCPs during catalysis. In this study, the catalyst through the in-situ reconstruction of the diazole CuCPs under electrochemical conditions has demonstrated excellent CO2RR performance with the C2+ products Faradaic efficiency of 80% at a current density of 1 A cm-2. In-situ Raman spectra indicated that the organic ligands promoted the high-frequency band linear *CO on the Cu surface which is related to the enrichment of cations at the interface. Compared with the triazole CuCPs, the increase proportion of K+ ion hydrated water facilitated the water dissociation process, leading to the transformation of the products from C2+ to methane and hydrogen. This work aims to clarify the role and significant functions of molecular in the reaction process, and provide spectroscopic evidence and theoretical guidance for the catalytic mechanism and reaction pathway of copper catalysts modified with organic.

References:

[1] Xu, Z., Lu, R., Lin, Z., Wu, W., Tsai, H., Lu, Q., Li, Y., Hung, S.*, Song, C., Yu, J., Wang, Z.*, Wang, Y*. Nat. Energy. 2024, 9: 1397.

[2] Du, Z., Li, S., Xie Y., A, Y., Zhang, Y., Zhang, H.*, Tian, J., Zheng, S.*, Zheng, Q., Chen, Z.*, Ip, W., Liu, J.*, Li, J*. J. Am. Chem. Soc. 2024, 146: 32870.

Keywords: CO_2 reduction reaction, Copper coordination polymers, In-situ Raman

[Abstract:0021] [SERS/TERS/Plasmonics]

Noninvasive Breath-Based Monitoring of Oxidative Stress Via Photoinduced Charge-Transfer Mechanisms

***Jingwen Zhou*[1], *Yichuan Kou*[2], *Yue Jiao Zhang*[3], *Jian Feng Li*[3]**

[1]*School of Life Sciences, Xiamen University, Xiamen, China*
[2]*College of Physical Science and Technology, Xiamen University, Xiamen, China*
[3]*College of Energy, Xiamen University, Xiamen, China*

Sensitive, noninvasive detection of oxidative stress is critical for early disease intervention and health monitoring, yet current methods often lack sufficient sensitivity and specificity. Surface-enhanced Raman scattering (SERS) provides a rapid, label-free approach for molecular fingerprinting, but its chemical enhancement potential remains largely untapped. In this study, we develop a photoinduced charge-transfer (PICT) resonance-enabled platform that synergizes charge-transfer and electromagnetic effects through precise excitation wavelength tuning. This design selectively amplifies target vibrational modes, resulting in a 100-fold increase in responsiveness toward gaseous aldehydes, which are key biomarkers of oxidative stress in exhaled breath, and achieves an extraordinary detection limit of 60 ppt. Coupled with a portable Raman device, this strategy allows clear differentiation of oxidative stress levels between healthy subjects and patients. Beyond advancing SERS sensitivity, our approach offers a practical, noninvasive solution for real-time health assessment and clinical biomarker analysis.

Keywords: surface enhanced Raman scattering (SERS), photoinduced charge transfer (PICT) resonance, noninvasive diagnosis, oxidative stress, gaseous aldehydes

[Abstract:0022] [Coherent Raman Imaging]

Doppler Dual-Comb Coherent Raman Spectromicroscopy and Holography

***Florian Matthias Schweizer*, Manish Garg**

Quantum Microscopy and Dynamics Group, Max Planck Institute for Solid State Research, Stuttgart, Germany

Label-free chemical imaging enabled by Raman spectroscopy has been a widely investigated topic in the last decades. Stimulated Raman spectroscopy (SRS) overcomes the major limitation of low sensitivity in spontaneous Raman spectroscopy, but at the cost of probing only narrow spectral bandwidths at a time. In contrast, time-domain dual-comb coherent anti-Stokes Raman spectroscopy (CARS) can probe a broad spectral range (~ 400-1500 cm^{-1}), but its implementation is strenuous owing to the difficulty associated with temporal synchronization of two broadband laser sources. In my talk, I will introduce a new time-domain coherent Raman spectroscopy method, utilizing the dual-comb approach with a single laser source, where the frequency shift in the comb is generated by the Doppler effect. Both the frequency combs impulsively excite vibrations in the sample, which interfere and periodically modulate their Kerr nonlinear response. The time varying Kerr nonlinear response leads to spectral broadening and periodic modulation in the anti-Stokes spectral regions of both the frequency combs. The Doppler frequency shift between the two frequency combs leads to a down-conversion of the vibrational frequencies, from ~100 THz to the MHz range, which allows the use of highly sensitive, but relatively slow single-photon counters. A broad range of samples, from liquids, wide bandgap dielectrics to micro-particles were investigated with non-damaging pulse energies (< 100 pJ). Furthermore, due to the high nonlinearity of the involved multiphoton processes, a spatial resolution way below the diffraction limit (~170 nm in lateral dimensions and ~10 nm in the axial dimension) was achieved.

Keywords: Coherent Raman, Broadband, Super-resolution, Spectro-imaging, Dual comb

[Abstract:0024] [SERS/TERS/Plasmonics]

Cost-Effective Plasmonic SERS Substrate Via Tunned Silver Mirror Reaction for Sensitive Herbicide Detection

***Raju Botta*, Khwanchai Tantiwanichapan, Pitak Eiamchai, Saksorn Limwichean, Noppadon Nuntawong, Mati Horprathum**

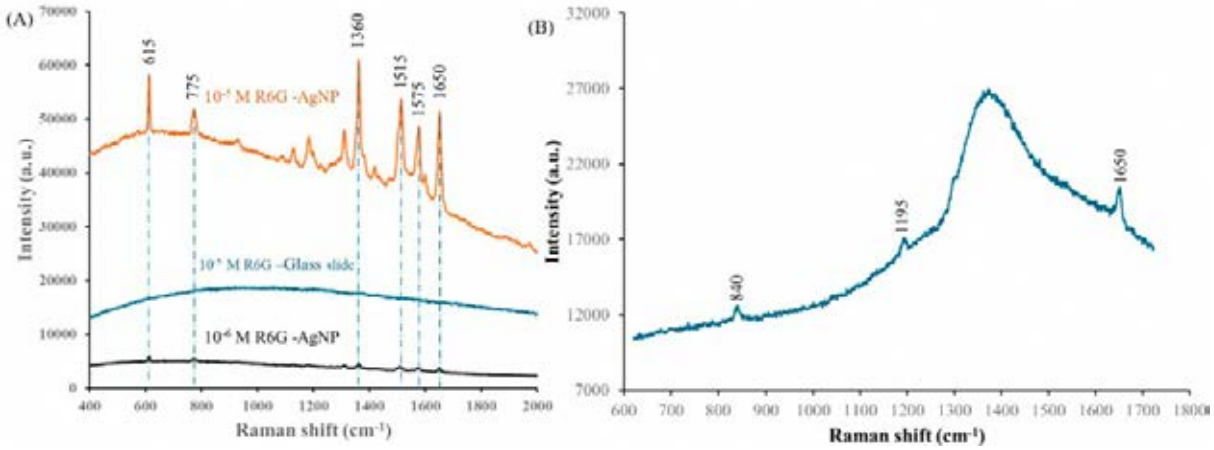
Spectroscopic and Sensing Devices Research Group (SSDRG), National Electronics and Computer Technology Center (NECTEC), Pathum Thani, Thailand

Rapid and sensitive detection of hazardous agrochemicals remain challenge in environmental and food safety monitoring. Surface enhanced Raman Spectroscopy (SERS) has emerged a power molecular fingerprinting technique for trace chemical detection due to its high sensitivity and specificity. However, fabrication of highly active SERS substrates often relies on sophisticated and costly nanofabrication methods such as physical vapor deposition (PVD), chemical vapor deposition (CVD), lithography, thermal evaporation, and laser ablation. These methods, although effective, limit large-scale and cost-effective deployment of SERS-based sensors. In this study, we report a facile and low-cost strategy for fabricating plasmonic SERS substrates by tuning the silver mirror reaction to get densely packed silver nanoparticles and nanoclusters (AgNPs/AgNCs) directly on glass slides.

The morphology and spatial distribution of the fabricated nanostructures were characterized using FESEM, revealing a uniform nanoparticle distribution across the substrate surface. Such distribution creates numerous interparticle nanogaps known as "hotspots", generates strong localized surface plasmon resonance (LSPR) and enhance the Raman signal significantly. The SERS performance of the fabricated substrate was evaluated using Rhodamine 6G (R6G) as a probe molecule at different concentrations. Characteristic Raman bands of R6G at 1650, 1575, 1515, 1360, 1310, 1185, 775, and 615 cm^{-1} were clearly observed even at lower concentrations, Figure 1A. A comparison of Raman spectra obtained at the same concentration on a bare glass slide and on the fabricated SERS substrate revealed an enhancement of approximately 142 times, demonstrating the strong plasmonic activity of the substrate. To demonstrate practical applicability, the developed substrate was employed for the detection of widely used paraquat (PQ) herbicide. Distinct Raman lines of PQ at 1650, 1195, and 840 cm^{-1} were successfully detected at a concentration of 10 μM, Figure 1B. The substrate also exhibited good signal reproducibility with relative standard deviation of 13% across locations on the substrate surface. These results demonstrate that controlled tuning of silver mirror reaction provides a simple and scalable route for producing sensitive and cost-effective plasmonic SERS substrates, offering promising potential for rapid environmental monitoring of hazardous agrochemicals.

Keywords: Plasmonics, Silver Nanoparticles, SERS, Herbicides,, Paraquat

Figure 1. SERS spectra of probe molecules on AgNP substrate: (A) R6G at different concentrations along with R6G Raman spectrum on glass slide and (B) 10 µM concentration of PQ.



[Abstract:0028] [SERS/TERS/Plasmonics]

Protein-Gold Nanoparticle Interface Characterized by Machine Learning-Assisted Surface Enhanced Raman Scattering (SERS)

***Shrobona Banerjee*[1], *Florian Gaerber*[2], *Stephan Seifert*[2], *Janina Kneipp*[1]**

[1]*Department of Chemistry, Humboldt-Universitaet zu Berlin, Berlin, Germany*
[2]*Department of Chemistry, Universitaet Hamburg, Hamburg, Germany*

The characterization and control of protein-gold nanoparticle interactions is important for theranostics and biotechnological applications. The protein-gold interface is of analytical importance because proteins are structurally diverse biomolecules involved in virtually all biochemical processes, while gold nanoparticles (AuNPs) have emerged as excellent materials for probing and modifying living systems due to their tunable optical properties, surface chemistry and biocompatibility.

Surface enhanced Raman scattering (SERS) using AuNPs as plasmonic substrates is an excellent technique for probing proteins in biological and biomimetic environments [Drescher et al., ACS Nano, 2021, 15(9), 14838–14849]. Since SERS is extremely sensitive to miniscule changes in the nanoscale environment, SERS spectra can provide insight into protein structure and protein-gold interactions at the immediate interface [Szekeres et al., Front. Chem., 2019, 7, 30]. Here, we shall show how SERS spectra of aqueous protein-AuNP mixtures could be used to distinguish between different proteins, based on varying structural motifs in the protein analyte as well as differing interactions between the protein and AuNP surface.

Despite being rich in spectral information, SERS show high variability and signal fluctuations. To deconvolute this complex spectral information, SERS spectra were analyzed with supervised learning techniques – support vector machines (SVM) and random forests (RF) – which were trained to discriminate SERS spectra of four different proteins – bovine serum albumin (BSA), lysozyme (LYSO), pepsin (PEP) and streptavidin (STREP). Both models demonstrated high classification accuracies and yielded explainable metrics – Support Vectors (SVs) from SVM, and Surrogate Minimal Depth (SMD) and Mean Adjusted Agreement (MAA) from RF [Feng et al., J. Phys. Chem. C, 2024, 128(46), 19722–19735]. The SVs identified critical spectral signatures while SMD discerned the most important vibrational modes which could be used to distinguish different classes of protein spectra. The MAA mapped the interdependence between different spectral bands, which could explain the co-occurrence or co-dependence of specific spectral features. Thus, the results of this multivariate analysis offer a unified lens on discriminative spectral features that can distinguish and characterize SERS spectra of different proteins.

Keywords: SERS, Proteins, Multivariate Classification, Chemometrics, Machine Learning

[Abstract:0029] [Coherent Raman Imaging]

Super-Broadband Stimulated Raman Scattering Spectroscopy and Imaging

Jin Guo, Qiaozhi Yu, Haojie Zhang, Jiakai Wang, Hanqing Xiong

National Biomedical Imaging Center, College of Future Technology, Peking University, Beijing 100871, China

Coherent Raman scattering (SRS) has emerged as a powerful quantitative contrast mechanism for chemical imaging in recent years. However, thanks to the high spectral quality of spontaneous Raman over large bandwidths, the very fundamental spontaneous Raman scattering still holds its superiority over CRS in simultaneously detecting a wide variety of biomolecules. In this talk, I will present a novel time-domain excitation strategy developed in our lab that provides identical spectra to the state-of-the-art spontaneous Raman over thousands of wavenumber ranges but is orders of magnitude faster in spectral acquisition speed. By encoding Raman free-induction decays into time-domain stimulated Raman loss (SRL) signals through few-cycle laser-induced quantum interference, we reconstruct the full-range Raman spectrum via Fourier transform of the time-domain SRL signal. This approach achieves natural-linewidth-limit spectral line shapes and enhanced sensitivity. I will discuss our progress in obtaining self-calibrated full-range Raman spectra and high-speed super-broadband Raman imaging, along with the advantages and limitations of this method for biomedical imaging applications.

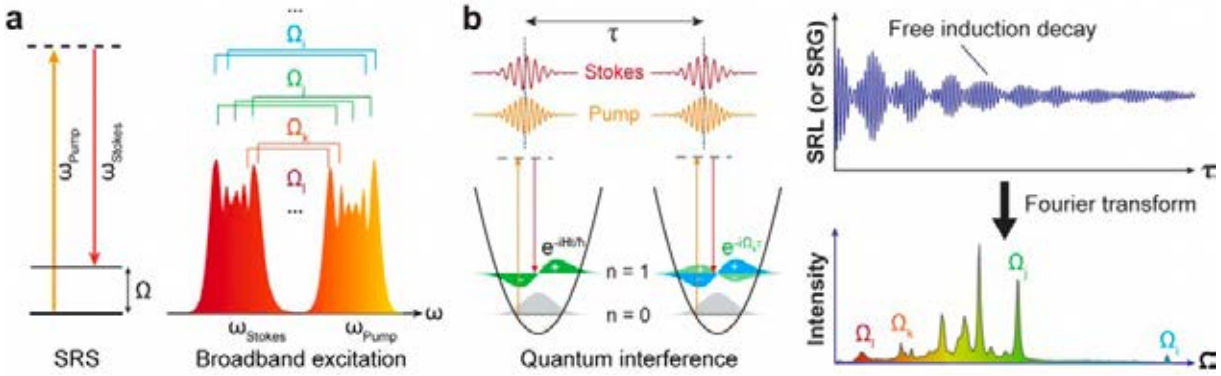
References:

1. Guo, J., Wang, M., Yu, Q. et al. Super-broadband stimulated Raman scattering spectroscopy and imaging. Nat. Photon. (2026). https://doi.org/10.1038/s41566-025-01841-8

2. Yu, Q., Yao, Z., Zhou, J. et al. Transient stimulated Raman scattering spectroscopy and imaging. Light Sci Appl 13, 70 (2024). https://doi.org/10.1038/s41377-024-01412-6

Keywords: stimulated Raman scattering, few-cycle laser pulse, quantum interference, free-induction decay, hyperspectral imaging.

Principle of super-broadband stimulated Raman scattering.



a, The excitations of many Raman modes simultaneously by broadband lasers. b, Principle of deciphering the spectra of many Raman modes by broadband impulsive excitations. The FIDs of many Raman modes are encoded into SRL (SRG) by quantum interference of the excited state probability amplitudes, and Fourier transform of the FIDs results in natural-linewidth-limited Raman spectra.

[Abstract:0030] [SERS/TERS/Plasmonics]

Controlling Gold Nanoparticles Electrodeposition for Reproducible SERS Substrates on Transparent Electrodes

***Ana Luiza Clivatti Yamanaka*, Rafael Da Silva Santos, Gabriel Negrão Meloni, Romulo Augusto Ando**

Laboratório de Espectroscopia Molecular, Instituto de Química, Universidade de São Paulo, São Paulo, Brasil

Electrodeposition of metallic nanoparticles (NPs) has emerged as an attractive strategy for the fabrication of SERS-active substrates. However, literature reports conflicting electrosynthesis protocols, particularly regarding applied potentials and deposition times, leading to inconsistencies in nanoparticle morphology and SERS performance. This work proposes a rational protocol for the electrodeposition of gold nanoparticles (AuNPs) on a transparent electrode, enabling the fabrication of an electroactive SERS platform suitable for spectroelectrochemistry investigations. A previously reported pulse-potential methodology for AuNPs formation1 was initially evaluated using indium tin oxide (ITO) electrodes. Scanning electron microscopy was employed to assess nanoparticle size and morphology, and SERS activity was subsequently investigated. Given the critical role of reproducibility in SERS measurements, the influence of ohmic potential losses associated with uncompensated resistances in the electrochemical cell2 was systematically considered. The electrodeposition procedure was therefore performed with and without ohmic-drop compensation based on experimentally measured resistance values. An electroactive probe molecule (potassium ferricyanide, 10-4 M) was selected since it exhibits SERS activity3 (Figure 1). Cyclic voltammetry of $HAuCl_4$ on ITO (Figure 2) reveals that the effective potentials required for nucleation and growth4 differ from those assumed in the reference protocol1. When compensating ohmic-drop (Substrate 1) the larger effective electrode potential drives faster AuNP growth, resulting in irregular morphology and oversized nanostructures, leading to poorly reproducible SERS substrate. In contrast, deposition without ohmic-drop compensation (Substrate 2) drives slow growth, yielding a more homogeneous nanoparticle distribution and improved SERS performance, as shown by potassium ferricyanide's enhanced spectroelectrochemical response (Figure 1). Although the procedure without ohmic-drop compensation resulted in better SERS substrate, uncompensated resistances may vary between experiments and the effective applied potential becomes unknown, resulting in irreproducible electrodeposition procedures. Building on these findings, we aim to systematically investigate the influence of ohmic-drop on nanoparticle electrodeposition at transparent electrodes by correlating compensated potential values, nucleation-growth dynamics, nanoparticle morphology, and SERS performance. This approach seeks to establish reproducible electrochemical criteria for electroactive SERS substrates rational design.

References:

1. Chem. Sci., 2019, 10, 936–942

2. Anal. Chem. 1996, 68, 1871-1876

3. J. Am. Chem. Soc. 2020, 142, 30, 13120–13129

4. Nanoscale, 2024, 16, 16204–16217

Keywords: SERS, gold, electrosynthesis, ITO, spectroelectrochemistry

Figure 1

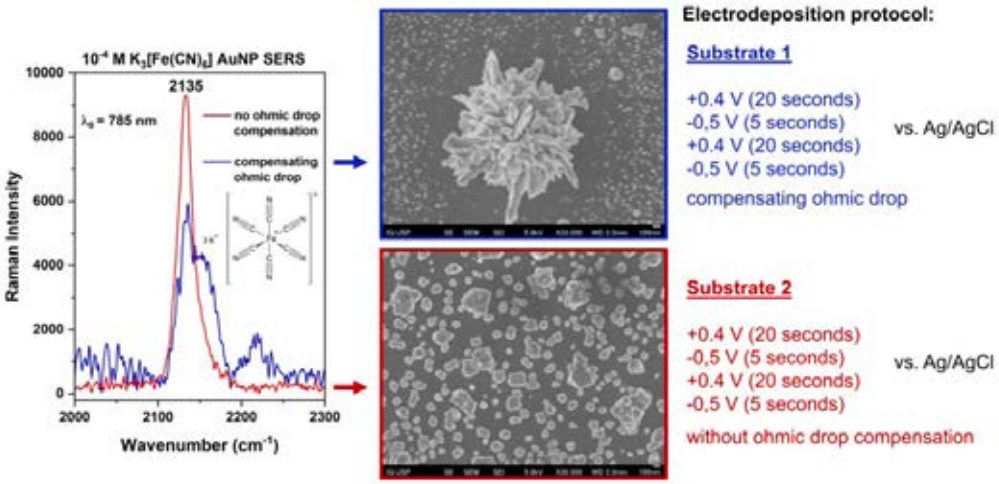


Figure 1: SERS response of 10^{-4} M potassium ferricyanide (λ_0 = 785 nm, 8 mW) recorded on the fabricated substrates with and without ohmic-drop compensation, together with the corresponding SEM micrographs.

Figure 2

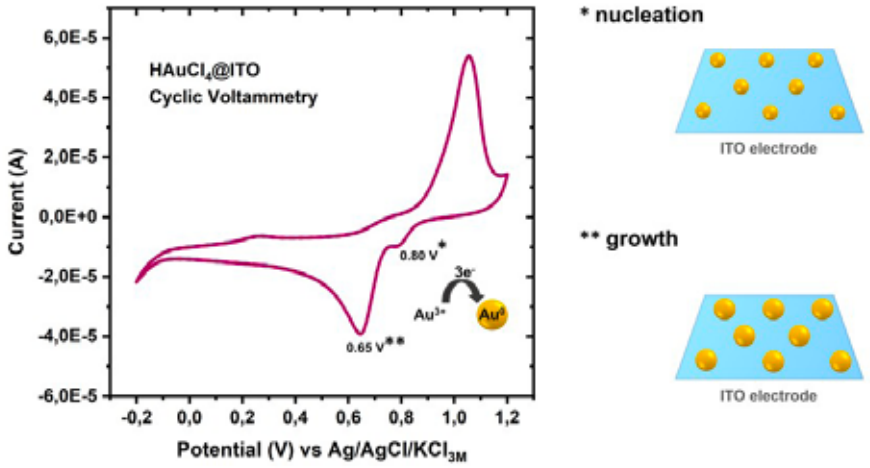


Figure 2: Cyclic voltammogram of 1 mmol L^{-1} $HAuCl_4$ recorded at 100 mV s^{-1} on an ITO electrode, using $LiClO_4$ as the supporting electrolyte, together with a schematic representation of the gold electrodeposition process.

[Abstract:0031] [Industrial/Societal Applications]

Deep-UV Resonance Raman Spectroscopy Enables Reliable MDMA Identification in Colored Ecstasy Tablets

Lars Jasperse[1], Merel C. Konings[1], Freek Ariese[1], Ruben F. Kranenburg[2]

[1]LaserLaB, Vrije Universiteit Amsterdam, Amsterdam, The Netherlands
[2]Team National Forensic Expertise (LFOX), The Netherlands Police, Driebergen, The Netherlands; Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, The Netherlands

In forensic drug enforcement, there is a growing need for rapid and accurate on-site analysis of illicit substances. Spectroscopic techniques, particularly Raman spectroscopy, are promising due to their molecular specificity and portability but its effectiveness is limited by fluorescence and colorant interference. In field casework, particularly with dark or brightly colored ecstasy tablets, fluorescence often obscures diagnostic Raman bands, leading to inconclusive or false-negative results.

We introduce resonance-enhanced deep-ultraviolet Raman spectroscopy (DUV-RRS) at 248.6 nm as a novel solution for selective MDMA detection in the fluorescence-free region. Using a recently commercialized NeCu laser source, an in-house DUV-RRS setup was constructed and benchmarked against a benchtop 785 nm Raman microscope and two handheld analyzers (TruNarc 785 nm, Pendar X10 830 nm SERDS), Figure 1. The DUV-RRS spectra of MDMA exhibits strong resonance enhancement of aromatic-ring vibrations around 1628 cm^{-1}, enabling sensitive and compound-specific detection even at 1 % w/w MDMA in pressed tablet mixtures. Distinct spectral shifts allow differentiation between MDMA, structural analogs (2,3-MDMA, MDEA, MDA), and cathinones such as methylone.

In a case study of 14 seized ecstasy tablets of various colors, MDMA was successfully identified in all samples using DUV-RRS, while conventional Raman systems failed for tablets containing dark, blue, or green pigments due to strong absorption, fluorescence, or colorant resonance enhancement. DUV-RRS thus eliminates the need for sample preparation or chemical extraction, offering rapid, unambiguous drug identification even in low-dose or inhomogeneous tablets. Although the current setup is semi-portable, recent advances in compact DUV laser technology make true handheld operation feasible in the near future.

This study demonstrates, for the first time, that resonance-enhanced DUV-RRS can address key limitations of existing portable spectroscopic tools, offering a promising step towards more reliable on-site drug identification in challenging forensic scenarios.

Keywords: deep-UV Raman, forensic drug detection, portable spectroscopy

Graphical abstract

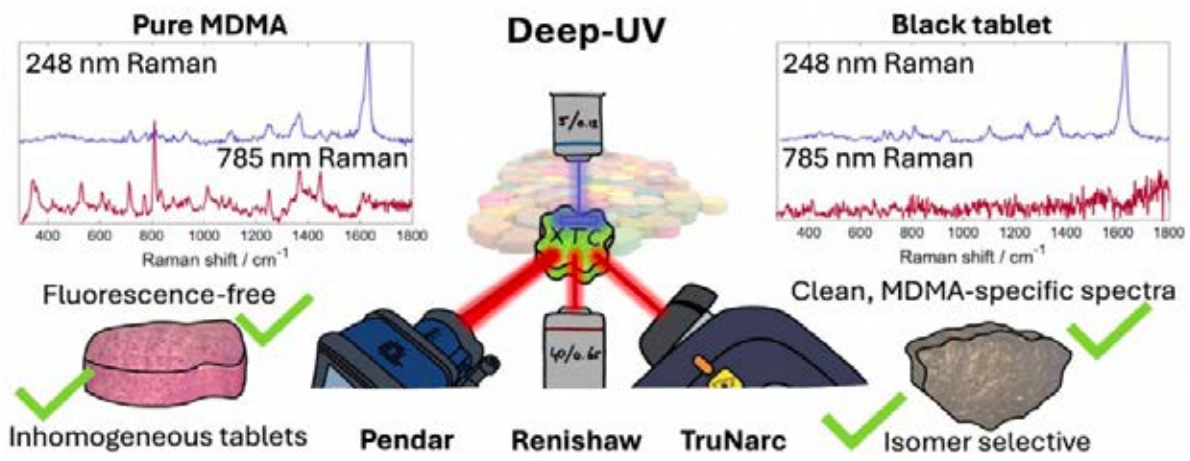


Figure 1. Schematic overview of the benchmark study of 248 nm deep-UV Raman against conventional Raman instruments. Graphical abstract, reprinted with permission from [For. Chem. 2025, 46, 100704]

[Abstract:0034] [SERS/TERS/Plasmonics]

Raman Spectroscopic of Single-Live-Cell Membrane Electrical Penetration Dynamics Via Plasmonic Nanotubes

***Yuge Liang*[1], *Peilin Xin*[1], *Jiaming Zhang*[3], *Yingqi Zhao*[1], *Jinglai Duan*[3], *Jinglai Duan*[4], *Jianan Huang*[1], *Jianan Huang*[2]**

[1]*Research Unit of Health Sciences and Technology, Faculty of Medicine, University of Oulu, Oulu, Finland, Biocenter Oulu, University of Oulu, Oulu, Finland*
[2]*Research Unit of Disease Networks, Faculty of Biochemistry and Molecular Medicine, University of Oulu, Oulu, Finland*
[3]*Institute of Modern Physics Chinese Academy of Sciences, Lanzhou, China, School of Nuclear Science and Technology, University of Chinese Academy of Sciences, Beijing, China*
[4]*Advanced Energy Science and Technology Guangdong Laboratory, Huizhou, China*

The demand for intercellular access into cells interiors is increasing but challenging due to conventional techniques failing to acquire information in real time and at single-cell resolution because of technical simplicity. The cell membrane hampering scientists to explore further that lysis reagents and membrane molecules present strong background that overlaps the analysis of the intracellular molecules of interests such as the mass spectrometry. Nanotechnology offers a transformative solution by enabling minimally invasive methods that penetrate cell membrane to continuously monitor intracellular activities, especially integrating with electricity depended on its precisely control, but the controversies on electropores formation still be remained. Here, we propose a plasmonic nanotube platform with the capacity of surface-enhanced Raman scattering (SERS) to monitor the membrane penetration dynamics of single-live gulfed cells in real-time via each 2-μm height, 100-nm diameter nanotube. These nanostructures have multifunction that can be applied 3.5-Vpp penetrated amplitude as nanoelectrodes and are allowed to deliver fluorescent dye into penetrated cellular interior.

Keywords: Plasmonic, SERS, Electroporation, Hollow structure, Single cell

Oral Abstracts

[Abstract:0036] [Biology/Biomedicine]

Monte Carlo Based Quantitative Spatially Offset Raman Spectroscopy Towards Non-Invasive Bone Quality Assessment

***Joseph O'Halloran*, Pranav Lanka, Jakub Byrdziak, Sanathana Konugolu Venkata Sekar, Stefan Andersson-Engels, Rekha Gautam**

Biophotonics@Tyndall, Tyndall National Institute, Cork, Ireland

Spatially offset Raman spectroscopy (SORS) shows significant promise as a noninvasive method for evaluating bone quality, as it can obtain biochemical information from bone through optically turbid biological tissue. Currently, bone health is assessed clinically using dual-energy X ray absorptiometry (DXA), which measures mineral density. Because SORS is sensitive to both the organic and mineral components of bone, it has the potential to provide diagnostically relevant information that complements DXA.

However, the highly scattering nature of biological tissue introduces considerable variability to SORS measurements, impeding accurate quantitative analysis based on Raman spectra alone. Instead, studies have focused on metrics such as band ratios and peak widths to form predictions of bone quality.

Here, we propose a novel approach using adjoint Monte Carlo (aMC) simulations (Figure 1) informed by optical properties extracted from time-of-flight (ToF) measurements. This allows us to account for the turbidity-induced Raman intensity variations and thereby enable quantitative analysis.

To understand the impact of optical turbidity, we developed an analytical framework to describe the Raman signal from a turbid sample and isolated a "light propagation factor" (LPF) that accounts for the turbidity effects. Prompted by this framework, we are using aMC simulations to calculate the LPFs for two sets of homogeneous tissue-mimicking phantoms. Subsequently, we will divide the experimentally measured Raman counts by the corresponding LPFs to recover linearity with analyte concentration. The first phantom set maintains a constant analyte concentration to assess turbidity correction. The second varies the analyte concentration to assess concentration-retrieval accuracy, using measurements of samples with known concentrations to generate a calibration curve.

To the best of our knowledge, this study presents the first Monte Carlo based method for quantitative SORS analysis. Although used here on homogeneous phantoms for simplicity and clarity, the approach is, in principle, readily scalable to more complex geometries, such as heterogeneous and multilayer geometries, given appropriate optical property estimates. As such, this study represents meaningful progress toward achieving precise, noninvasive Raman-based evaluation of bone quality.

Acknowledgments:

This work is conducted with the financial support of Taighde Éireann—Research Ireland Professorship (SFI/22/RP-2TF/10293) and Pathway (24/PATH-S/12518) grants.

Keywords: spatially offset Raman spectroscopy, bone, Monte Carlo, quantification, optical properties

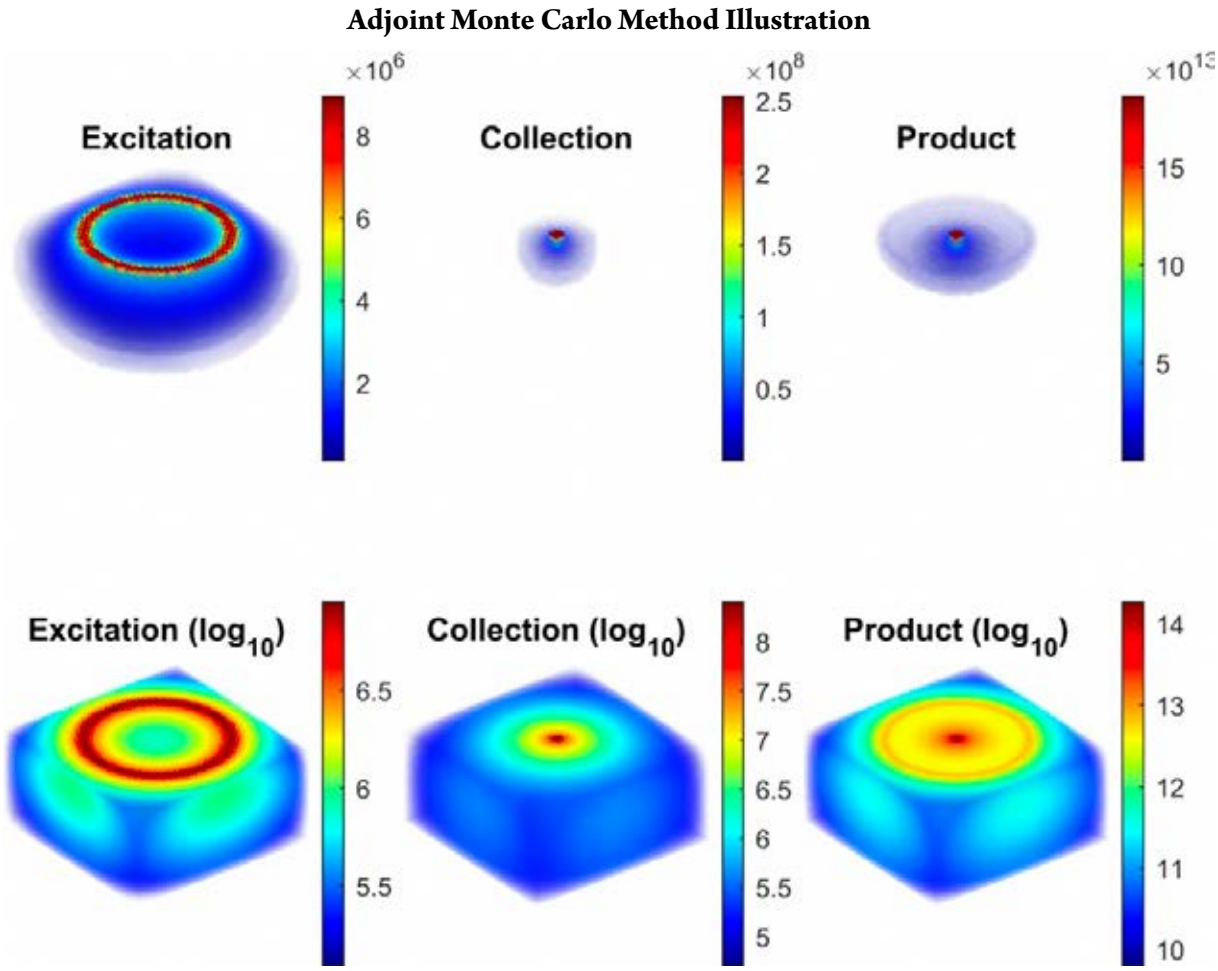


Figure 1: Illustration of adjoint Monte Carlo method: simulated photon fluence from source (Excitation) is multiplied by photon fluence from detector (Collection), and the value at each voxel in the resultant volume (Product) is summed together to generate the light propagation factor.

[Abstract:0037] [Coherent Raman Imaging]

A Self-Calibrated High-Speed Delay Scanning System for Time-Domain Stimulated Raman Spectroscopy

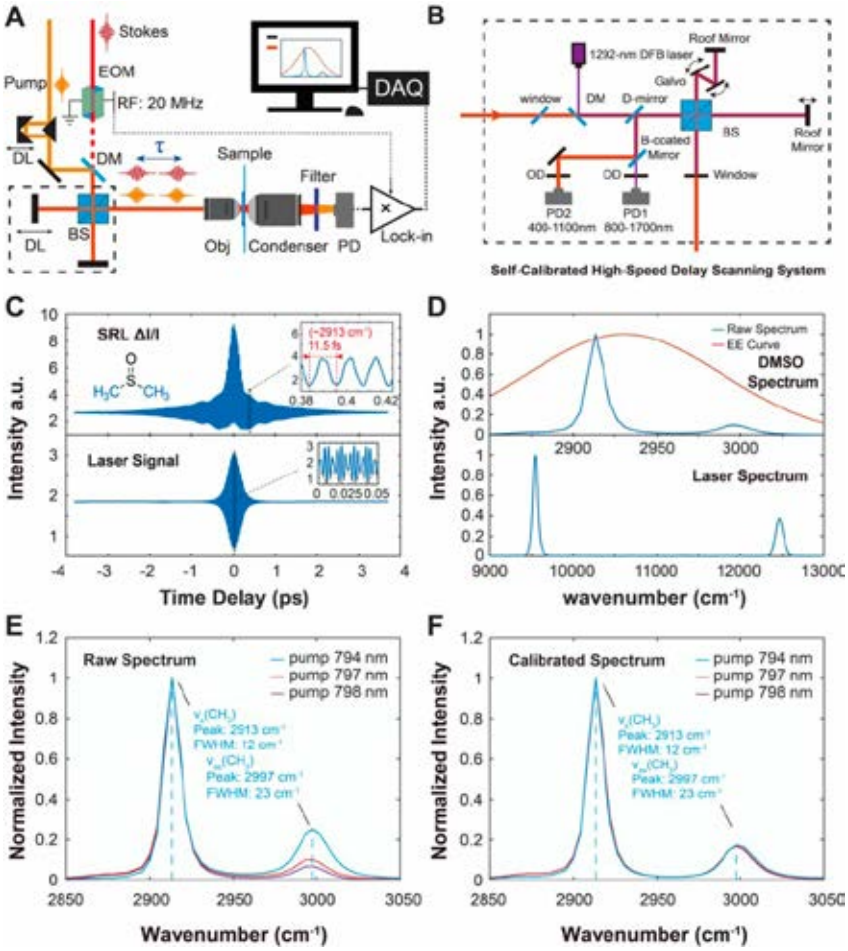
Jin Guo, Haojie Zhang, Hanqing Xiong

National Biomedical Imaging Center, College of Future Technology, Peking University, Beijing, China.

We present a self-calibrated high-speed delay scanning system for transient stimulated Raman scattering (T-SRS) spectroscopy. Inheriting the autofluorescence rejection of conventional SRS, T-SRS achieves quantum-limited spectral line shapes. Here, we further enhance it with hardware-based self-calibration that corrects spectral distortions from excitation drift, using an all-plane-mirror Michelson interferometer and a narrow-linewidth DFB reference laser for real-time calibration. Validated on dimethyl sulfoxide (DMSO) and further applied to label-free T-SRS imaging of epithelial tissue, the system consistently recovers accurate Raman signals—restoring protein- and lipid-rich spectra to benchmark profiles after calibration. This approach ensures long-term spectral fidelity for quantitative chemical imaging and time-domain spectroscopy.

Keywords: Self-Calibrated,stimulated Raman scattering, time-domain

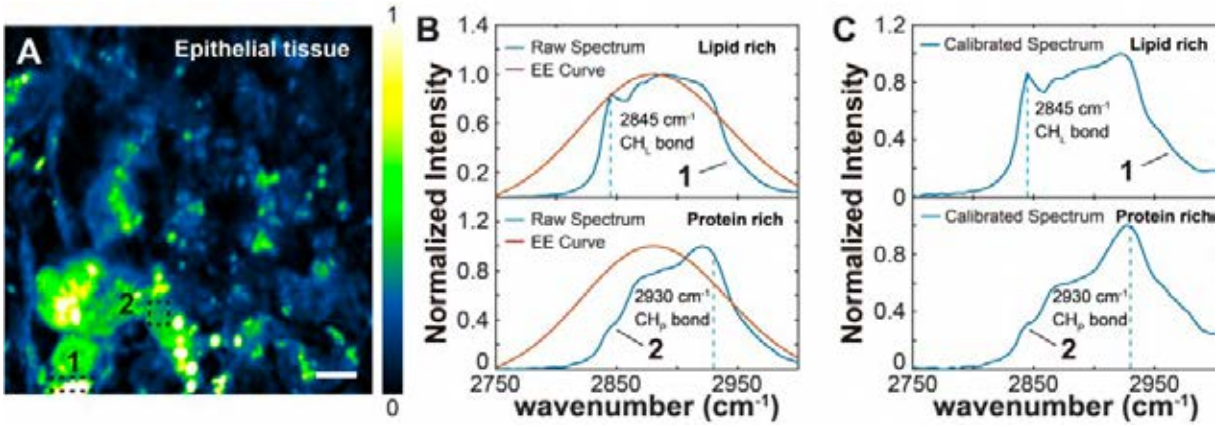
Self-calibrated transient-stimulated Raman scattering (T-SRS).



(A) Setup of T-SRS spectroscopy. EOM for electro-optic modulator; DL for delay line; DM for dichroic mirror;

BS for beam splitter; PD for photodiode; Obj for objective; DAQ for data acquisition card. (B) The detailed interferometer module (i.e., the dashed box region in (A)). OD for optical density filter. (C) The upper panel shows the time-domain stimulated Raman loss (SRL) signal of C–H stretching modes of dimethyl sulfoxide (DMSO) under T-SRS excitation and the lower panel shows the interference fringe of the excitation lasers (pump and Stokes). (D) The corresponding Fourier transform of the time-domain signal in (C). EE curve for excitation efficiency curve. (E) Raw T-SRS spectra of C–H stretching modes of DMSO with pump pulse wavelengths centered at 794, 797, and 798 nm, respectively. (F) The self-calibrated spectra of the corresponding raw spectra shown in (E).

Self-calibrated T-SRS imaging of the epithelial tissue in the C–H stretching band.



(A) T-SRS image of the epithelial tissue. (B) Raw spectra and EE curve of the selected region, "1" is for the lipid-rich region and "2" is for the protein-rich region. (C) Calibrated spectra of the lipidrich region and protein-rich region. Scale bar: 10 μm.

[Abstract:0039] [SERS/TERS/Plasmonics]

Validated Quantitative SERS Method for Trace Pharmaceutical Detection

***Shathar Alobeidat*[1], *Chiara Bezze*[2], *Nicola Fin*[2], *Alois Bonifacio*[1]**

[1]*Department of Engineering and Architecture, University of Trieste, Trieste, Italy*
[2]*F.I.S. Fabbrica Italiana Sintetici SpA, Vicenza, Italy*

Surface-enhanced Raman Spectroscopy (SERS), is a powerful spectroscopic technique characterized by its amplification of signature Raman signals using plasmonic nanostructures, attaining sub-nanomolar detection limits of target analytes. This study presents a validated SERS-based analytical method for the rapid detection of active pharmaceutical ingredients (APIs) with high sensitivity below 1 ppb, significantly reducing analysis time of conventional analytical methods. Design of Experiments (DoE) approaches were used to investigate SERS signals obtained using multiple plasmonic nanostructures as SERS substrates. Quantitative analysis was carried out using linear regression modeling of SERS peak intensities and validated through binary classifications of independent samples. The validated SERS method presented herein offers a rapid, sensitive and cost-effective approach for monitoring trace pharmaceutical contamination in complex matrices.

Keywords: Surface-enhanced Raman Spectroscopy (SERS), Plasmonic Nanoparticles, Quantitative Analysis, Trace Detection

[Abstract:0041] [Coherent Raman Imaging]

Intrinsic Backward Emission of Coherent Raman Photons From Homogeneous Media

Sandro Heuke, Jitendra Acharyya, Gina Benni, Anne Sentenac, Hervé Rigneault

Aix Marseille University, CNRS, Centrale Med, Institut Fresnel, 13013 Marseille, France.

Same-side (epi) detection is essential for coherent Raman microscopy whenever transmission is impractical, such as in thick, scattering tissues or endoscopic geometries. Yet, in homogeneous media, coherent Raman signals are generally emitted predominantly in the forward direction; measurable backward light often relies on interfaces, disorder, or multiple scattering, which compromises refocusing and spatial specificity. Here we show that this limitation can be overcome by exploiting momentum conservation in a four-wave-mixing process: with an appropriate choice of wavelengths and tight focusing, coherent Raman photons can be generated intrinsically into the backward half-space, without requiring structural inhomogeneity.

We implement this concept using coherent Stokes Raman scattering (CSRS), where the emitted wavelength is red-shifted into the visible range. Combining vectorial, k-space-based modeling with experiments, we identify the conditions that maximize backward CSRS—highlighting the role of high-NA focusing, non-paraxial wave-vector components, and polarization states that enhance backward phase matching. The simulations provide practical design rules for pupil-plane beam shaping and for balancing forward and backward emission.

Experimentally, we observe a pronounced backward CSRS component from liquids and from optically challenging biological specimens under tight focusing. The backward signal remains focal and coherent, supporting imaging configurations that collect the nonlinear response from the same side as excitation. These results establish CSRS as a compelling route toward efficient epi-detected coherent Raman microscopy, and open opportunities for thick-sample imaging, compact implementations, and endoscopy-oriented architectures.

Keywords: Coherent Raman imaging, Coherent Stokes Raman imaging (CSRS), Backscattering

[Abstract:0043] [Theory/Computation]

Evaluating And Choosing Experimental Parameters For Shifted Excitation Raman Difference Spectroscopy: A Quantitative Study

***Jesper Sand*[1], *Minna Grønning Jensen*[2], *Erik Skibsted*[3], *Anders Kristensen*[1]**

[1]*Department of Health Technology, Technical University of Denmark, Kgs. Lyngby, Denmark*
[2]*CMC Analytical Support, Novo Nordisk A/S, Måløv, Denmark*
[3]*PAT and Statistics, Novo Nordisk A/S, Måløv, Denmark*

Shifted excitation Raman difference spectroscopy (SERDS) is an efficient method for rejecting fluorescence backgrounds in Raman spectroscopy. However, the technique lacks simple guidelines for selecting key experimental parameters, and quantitative tools to predict how the choice of parameters affects the results. In particular, the choice of excitation wavenumber shift, δ, and acquisition frequency, f, influences the accuracy, signal-to-noise ratio (SNR), and background rejection capability of the SERDS method.

In this work, we provide a quantitative framework for understanding and optimizing these parameters to support reproducible and application-adapted SERDS measurements by deriving and experimentally validating theoretical formulas.

We first analyze the spectral distortion introduced when employing a non-negligible magnitude of the wavenumber shift. Because SERDS is based on subtracting two spectra displaced in wavenumber, the resulting difference spectrum deviates systematically from the analytical first derivative of the Raman signal, as illustrated in Figure 1. For a Gaussian peak, we derive an explicit expression quantifying this deviation as a function of δ and Full-width-at-half-maximum (FWHM), establishing conditions under which derivative-like behavior is well approximated.

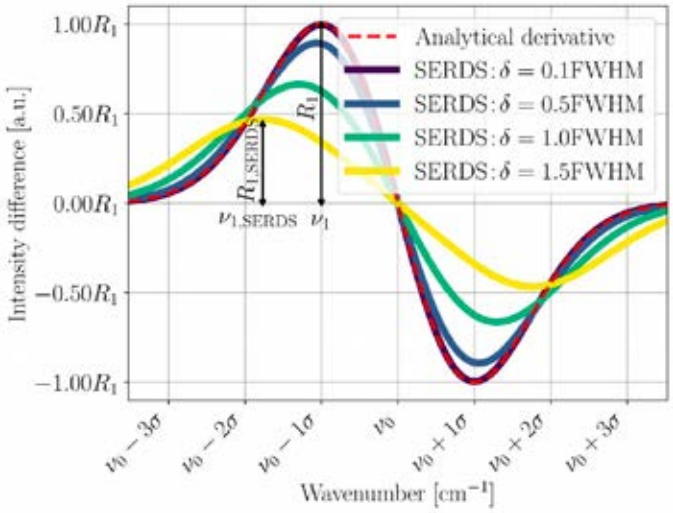
Secondly, we investigate how the SNR of SERDS spectra depends on the magnitude of the applied wavenumber shift. By modeling the noise and evaluating peak heights as a function of δ and linewidth, we provide a formula to quantify the SNR. All formulas are compared to measurements of polystyrene, as exemplified in Figure 2.

Based on the analysis, we propose a practical guideline: for applications requiring quantification or high reproducibility, an optimal shift is approximately $\delta \approx (1/2)\cdot$FWHM_min or less, where FWHM_min is the linewidth of the narrowest peak of interest. In contrast, for simple analyte presence detection on top of a strong fluorescence background, larger shifts can be advantageous to improve SNR. However, we show that SNR plateaus beyond a certain magnitude of δ.

Finally, we address samples affected by time-dependent signal changes such as photobleaching. We provide an estimate of the repetition frequency required to minimize artifacts in averaged SERDS spectra recorded in series, and quantify the photobleaching-induced error. The formula is compared to measurements of polyetheretherketone (PEEK), as shown in Figures 3 and 4.

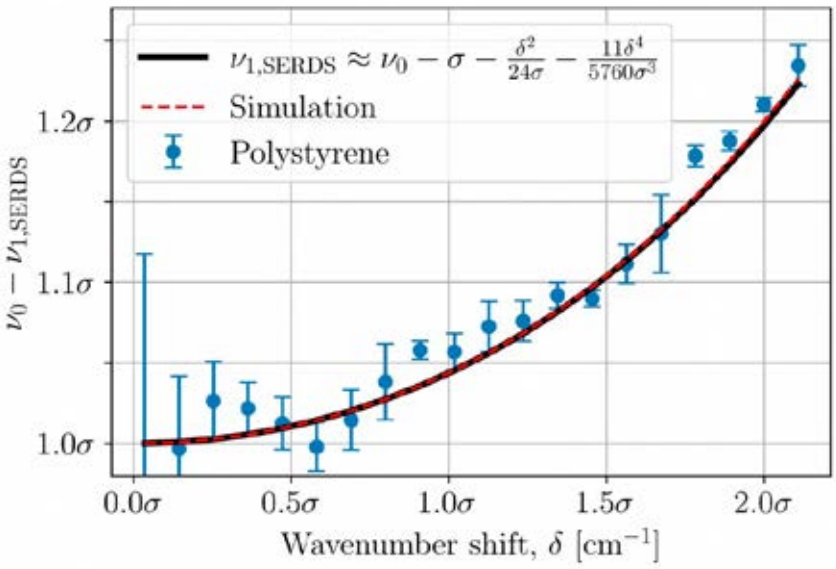
Keywords: SERDS, shifted, excitation, difference, Raman, spectroscopy

Figure 1: SERDS spectra for varying wavenumber shifts



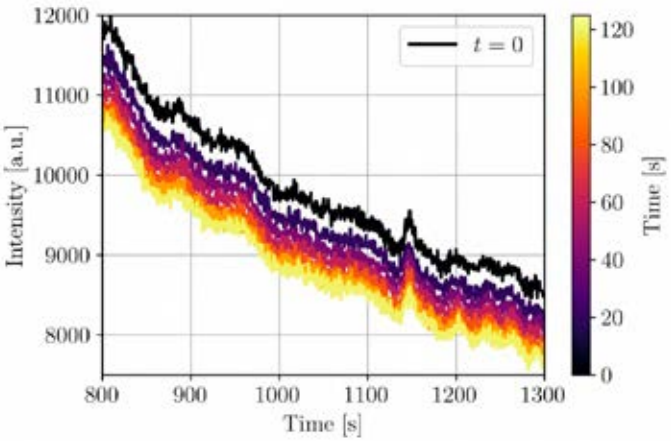
Displays the parameters of the resulting SERDS spectra for varying wavenumber shifts, δ. The spectra are obtained by taking the difference spectrum of two Gaussian profiles shifted by δ relative to one another. As evident from the figure, the resulting peak height, R1_SERDS, and peak position, v1_SERDS, deviate from the corresponding values of the analytical Gaussian first derivative, R1 and v1.

Figure 2: Experimental comparison with polystyrene



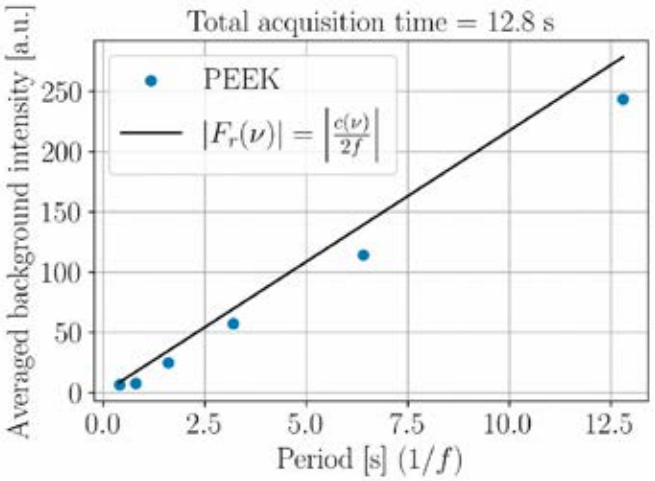
Displays the theoretical, simulated, and measured values of v1_SERDS, as defined in Figure 1. The theoretical formula is shown in the legend. The simulated values were obtained by constructing SERDS spectra from ideal Gaussian profiles. The experimental values were obtained from SERDS spectra measured of the major polystyrene peak at 1001 cm^-1.

Figure 3: Photobleaching of polyetheretherketone (PEEK)



Displays spectra recorded of polyetheretherketone (PEEK) at different timestamps. As evident from the figure, the intensity decreases over time due to photobleaching.

Figure 4: Photobleaching-induced error as function of repetition frequency



Displays the predicted upper bound on the magnitude of the resulting background, F_r, of averaged SERDS spectra obtained with varying repetition frequency, f. The corresponding measured values were obtained from averaged polyetheretherketone (PEEK) SERDS spectra. c(v) is the slope of a linear fit to the intensity versus time at wavenumber v during the initial stage of the bleaching process.

[Abstract:0047] [Materials]

Insights İnto Synthesis of Metal-Organic-Frameworks (MOFs) with Combined In Situ Approach: Raman Scattering, X-Ray Absorption and X-Ray Diffraction

***Olena Zavorotynska*[1], *Sofiia Bercha*[1], *Sachin Chavan*[2]**

[1]*Department of Mathematics and Physics, University of Stavanger, Stavanger, Norway*
[2]*Department of Chemistry, Bioscience and Environmental Engineering, University of Stavanger, Stavanger, Norway*

Metal–organic frameworks with a Zr-oxo cluster [(Zr6O4(OH)4)]12– are exceptionally stable and offer vast potential for a wide range of applications. Synthesis parameters strongly affect the quality, stability, morphology, etc., of the MOFs calling for elucidating of the various reaction steps.

We present a combined approach of three in situ techniques: powder X-ray diffraction (PXRD), X-ray absorption (XAS), and Raman spectroscopy (RS), that allows for integrated monitoring of MOF synthesis in different solvents and at variable temperatures. In the early pre-crystalline synthesis phase, the local (~2–5 Å) environment around Zr4+ ions and the Zr-oxo cluster formation is addressed by element-specific X-ray absorption at Zr k-edge. RS provides evidence of coordination between inorganic and organic blocks in the synthesis reaction. Owing to week scattering from water, RS is much more suitable for the in-situ studies of the water-based synthesis than infrared spectroscopy. Crystallization onset of the MOFs was evidenced by the appearance of the scattering peaks in the in situ patterns.

The kinetics of the various steps of the synthesis reaction can be studied using linear combination fits (LCS, X-ray absorption data), growth of PXRD reflections, and the intensity growth of the cluster–linker coordination vibrational mode [1]. The dependence of the reaction kinetics on water, modulator concentrations, solvent, and metal precursor were studied as well. The results of the in-situ experiments were correlated with post-synthetic characterization of the resultant MOF products [2].

References:

[1] S. Bercha et al. ACS Omega 2024, 9, 44, 44321-44335.

[2] Zavorotynska et al., Phys. Chem. Chem. Phys. 2024, 26, 27019-27033.

Keywords: MOF synthesis, in situ monitoring, multi-technique study, Zr-fumarate

[Abstract:0048] [SERS/TERS/Plasmonics]

Looking Beyond Gold and Silver, Quest for Inexpensive But Efficient SERS Substrates in Sandwich Immunoassays with SERS Readout and SERS for Detection of Proteinuria

***Rostislav Bukasov*[1], *Saule Mergenbayeva*[1], *Ansar Seitkali*[1], *Abduzhappar Gaipov*[2]**

[1]*Department of Chemistry, SSH, Nazarbayev University*
[2]*Department of Medicine, School of Medicine, Nazarbayev University*

SERS is area of sustained interest of a few 100s or research groups worldwide but practical applications of this technique in analysis are not nearly so numerous. Typically, substrate for SERS are made of gold or silver films or/and nanostructures, however, those may suffer from contamination by S-containing compounds and corrosion. Substrate, which is far less expensive and much more universally available in comparison to gold is Al foil. Also, it is passivated with several nm thick layer of Al2O3 and thus may be more stable and less susceptible to contamination. Therefore, Al foil may make SERS more attractive for variety of real-life applications in chemical analysis. One research areas is about direct SERS of urine for diagnostics of proteinuria, effect of substrate and gold nanoparticle size on its performance. The second direction is study of SERS enhancement as a function of nanoparticle association in dimers and trimers, which may be significant in many SERS assays. We did it at various substrates (Au film, Al, Si) and various interparticle distances by combining Raman and AFM maps or Raman and SEM maps, using a new method of map combination. The third direction of our group experimental research is SERS sandwich assays of biomarkers. We found that Al foil and Si could outperform gold film as a substrate in terms of selectivity in detection of human IgG, while they provide about the same or even better LOD, since the relative standard deviation of the blank for assays on Al foil and especially Si is typically better than those in the assays on gold film. Prior to SERS detection of clusterin we also used fluorescently tagged antibodies for selection of the substrate (among Au, Al foil and Si) and optimization of its parameters. Overall, we could detect human IgG with LOD 2 pM (20 attomoles in 10 microliter volume), as well as biomarkers MPT64 and clusterin with LOD 2 and 3 ng/mL respectively, while using Al foil, bought in the supermarket as a surface of SERS substrate for the immunoassay. In this talk we report developments in all 3 of those directions.

Keywords: SERS, SERS immunoassay, detection of biomarkers, Al foil, Structure-Activity Relationships

[Abstract:0049] [Coherent Raman Imaging]

Stimulated Raman Scattering Imaging of Dislocation-Induced Strain Fields in Bulk GaN Substrates

***Shun Takahashi*[1], *Yusuke Wakamoto*[1], *Kazuhiro Kuruma*[2], *Takuya Maeda*[1], *Yasuyuki Ozeki*[1]**

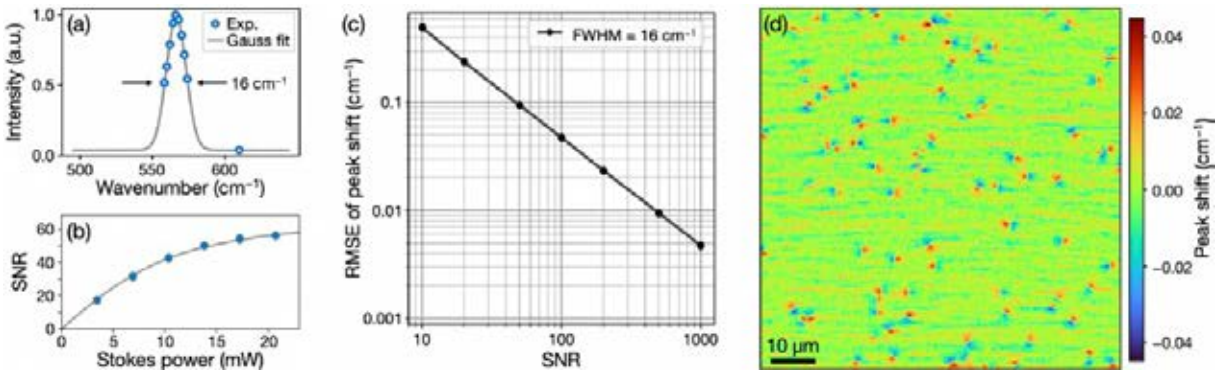
[1]*Department of Electrical Engineering and Information Systems, The University of Tokyo, Tokyo, Japan*
[2]*Research Center for Advanced Science and Technology, The University of Tokyo, Tokyo, Japan*

Gallium nitride (GaN) is a promising wide bandgap semiconductor for high-breakdown voltage, low-loss power devices. A vertical power device taking advantage of the material properties requires a high-quality GaN substrate, but GaN substrates typically contain numerous threading dislocations (TDs) with a density of 10^6 cm^{-2}. To reduce TDs that deteriorate the device performance, it is crucial to establish a characterization method capable of detecting them. Stimulated Raman scattering (SRS) microscopy has begun to be applied in materials science. Among its applications to crystalline materials, some studies focused on SRS peak shifts that reflected crystal strain and were >0.1 cm^{-1}. In this work, we realize SRS imaging of TDs in GaN substrates that induce strain fields and tiny peak shifts on the order of 0.01 cm^{-1}, which are several times smaller than previous reports, by carefully evaluating our imaging system and the requirements for TD detection.

As shown in Fig. 1(a), a peak wavenumber is derived by Gaussian fitting of SRS spectral data of GaN. The full-width at half-maximum of the spectrum is 16 cm^{-1}. Figure 1(b) shows the measured signal-to-noise ratio (SNR) of our pump-beam-detected SRS imaging system as a function of Stokes power. In this experiment, SRS signals were collected at a peak wavenumber with a dwell time of 4 μs. The saturated SNR with increased pump and Stokes powers was 55–65. We then numerically simulated the relationship between the SNR of signal detection and the root mean square error of derived peak wavenumbers (Fig. 1(c)). Based on these experimental and simulation results, we set the number of integration and spatial averaging for SNR improvement to 15 frames and 5 x 5 pixels, respectively. Figure 1(d) shows an SRS image of the local peak shifts of a GaN substrate. Many patterns consisting of a positive and negative peak shift pair visualize the TD-induced strain fields, while horizontal lines are due to system fluctuations. The effective pixel dwell time is 600 μs, and the standard deviation in the background is 0.005 cm^{-1}. This imaging result underscores the high speed and sensitivity of our SRS method to characterize TDs.

Keywords: stimulated Raman scattering microscopy, strain fields, gallium nitride, dislocations

Figure 1



(a) SRS spectrum of GaN. (b) Measured SNR of our imaging system as a function of Stokes power. (c) Numerical simulation of the relationship between SNR and root mean square error (RMSE) of peak shifts. (d) Mapping of SRS peak shifts induced by TDs.

Oral Abstracts

[Abstract:0050] [SERS/TERS/Plasmonics]

Biomedical and Analytical Applications of SERS Supported by Machine Learning: Towards Development of the Novel Tool for Clinical Diagnosis

***Agnieszka Kamińska*[1], *Sylwia Berus*[1], *Aneta Kowalska*[1], *Marta Czaplicka*[1], *Tomasz Szymborski*[1], *Wojciech Kukwa*[2], *Zuzanna Gronkiewicz*[2]**

[1]*Institute of Physical Chemistry Polish Academy of Science, Warsaw, Poland*
[2]*Otolaryngology Department of the Dentistry Division, Czerniakowski Hospital, Warsaw, Poland*

Surface–enhanced Raman spectroscopy provides a unique vibrational signature of the molecules under study. SERS, as an ultrasensitive, label-free, and non-destructive technique, reveals specific molecular-level information and thus offers valuable insights for biological systems analysis and monitoring. Plasmonic nanostructures based on femtosecond laser-modified Si (SERS platforms) have been developed to amplify the Raman signal of biological systems, with sensitivity, selectivity, and signal repeatability optimized. These SERS platforms were modified to be dedicated to specific applications, taking into account (i) the type of sample being tested (organic and inorganic analyses with sizes on the nanometer scale, eukaryotic and prokaryotic cells, tissues), (ii) and the form of tested samples (physiological fluids, swabs, homogenates). As examples of applications based on SERS platforms, chemometric analyses, microfluidic systems, and dielectrophoresis-based separation of biological systems, several sensors have been developed, including for the detection and identification of bacteria. These sensors exceed standard identification methods (biochemical, immunological, and molecular) in terms of simplicity, analysis cost, specificity, and speed of results. The combination of SERS-active nanostructures (Si/Ag), metal nanoparticles: magnetic nanoparticles (Fe2O3@Ag-NPs), and bimetallic Au@Ag-NPs allowed the development of two intrinsic (label–free) SERS configurations for tumor analysis in biofluids (e.g., blood, pleural effusion, urine, saliva) and in solid samples, and extrinsic SERS configuration for quantitative and qualitative analysis of biomarkers in biofluids. SERS-label imaging was adopted for solid tumor analysis. Coupling plasmonic nanostructures with microfluidic systems enables the miniaturization of the developed methods for their further point-of-care applications.

Keywords: SERS, microfluidic, dielectrophoresis, bacteria, cancer, chemometric

[Abstract:0057] [Coherent Raman Imaging]

Time-Lapse 3D SRS Imaging of Multicellular Systems with Reduced Photodamage Using Chirped Picosecond Pulses

***Itsuki Yamamoto*[1], *Kenta Temma*[2], *Kota Koike*[2], *Katsumasa Fujita*[1]**

[1]*Department of Applied Physics, The University of Osaka, Suita, Japan, Life-omics Research Division, Institute for Open and Transdisciplinary Research Initiatives, The University of Osaka, Suita, Japan*
[2]*Department of Applied Physics, The University of Osaka, Suita, Japan*

Multicellular systems such as spheroids and organoids provide physiologically relevant models for development, disease progression, and drug response because they preserve cell–cell interactions, spatial heterogeneity, and emergent tissue-like architectures that are not captured in 2D culture. To fully exploit these models, however, imaging methods must resolve dynamic processes in 3D over time while minimizing perturbation to native cellular behavior. Examples of biologically informative readouts include collective cell migration trajectories, proliferation and death dynamics, lumen or layered structure formation, and spatiotemporal heterogeneity in metabolic states or drug responses.

Stimulated Raman scattering (SRS) microscopy is well suited to this task because it provides label-free, chemically specific contrast based on molecular vibrations and enables volumetric imaging through intrinsic optical sectioning. In addition, unlike coherent anti-Stokes Raman scattering (CARS), SRS is not distorted by nonresonant background, which improves signal-to-background ratio for quantitative observation of living samples. However, repeated volumetric acquisition can still induce nonlinear photodamage because SRS relies on intense pulsed excitation.

Here, we present a spectral focusing SRS (SF-SRS) microscope using chirped picosecond pump and Stokes pulses to reduce photodamage during repeated 3D imaging. Spectral focusing in picosecond SRS has previously been shown to extend pulse duration from 2 ps to approximately 14 ps while maintaining 2 cm^{-1} spectral resolution and reducing excitation peak power, thereby suppressing damage in live-cell imaging [*Biomed. Opt. Express* 2022, 13, 995–1004]. Building on this concept, we implemented sectioning-based volumetric SRS imaging and applied it to time-lapse 3D imaging of living cells and to 3D imaging of living spheroids. These results demonstrate that chirped-pulse SF-SRS is a practical platform for longitudinal, label-free, chemically informative imaging of multicellular systems with reduced photodamage.

Keywords: Stimulated Raman scattering, Spectral focusing, 3D imaging, Time-lapse imaging

[Abstract:0060] [SERS/TERS/Plasmonics]

A Multi-Scanning-Probe Study of Local Nanoscale Properties in Cu-Doped Sb_2Se_3 Photovoltaic Films

***Giulia Spaggiari*[1], *Siiri Bienz*[2], *Renato Zenobi*[2], *Stefano Rampino*[1], *Naresh Kumar*[2], *Davide Calestani*[1]**

[1]*Istituto dei Materiali per l'Elettronica e il Magnetismo, Consiglio Nazionale delle Ricerche (IMEM-CNR), Parma, Italy*
[2]*Department of Chemistry and Applied Biosciences, ETH Zurich, 8093 Zurich, Switzerland*

This study investigates copper-doped antimony selenide (Sb_2Se_3) thin films, a promising photovoltaic absorber, at the nanoscale using conductive atomic force microscopy (C-AFM), tip-enhanced Raman spectroscopy (TERS), and Kelvin Probe Force Microscopy (KPFM). Although relatively high Cu concentrations (3–5 at.%) are used to achieve effective p-type doping, their nanoscale distribution and influence on local electronic properties remain unclear.

C-AFM measurements show that Cu doping increases film conductivity by nearly two orders of magnitude compared to undoped Sb_2Se_3. The current distribution is uniform at the microscale, with no evidence of preferential conduction along grain boundaries. However, ultra-thin doped films exhibit localized intra-grain conductivity hotspots, suggesting nanoscale dopant accumulation. These features are absent in thicker, device-relevant films, indicating a more homogeneous dopant distribution during growth.

TERS provides chemical insight into these observations. While confocal Raman spectroscopy detects micrometre-scale regions of the secondary phase $CuSbSe_2$, TERS reveals nanoscopic $CuSbSe_2$ inclusions as small as 50 nm embedded within the Sb_2Se_3 matrix. AFM and TERS mapping shows no preferential segregation of this secondary phase at grain boundaries.

KPFM links these structural features to electronic properties. The work function increases from 5.06 eV in undoped films to 5.21 eV in the Cu-doped Sb_2Se_3 matrix, confirming successful p-type doping. $CuSbSe_2$ inclusions exhibit an even higher work function (5.39 eV), indicating localized band bending that may affect charge-carrier dynamics.

Overall, the combined use of C-AFM, TERS, and KPFM provides detailed insight into nanoscale Cu doping in Sb_2Se_3. While high-concentration doping significantly enhances macroscopic conductivity, it also promotes the formation of secondary-phase nanocrystals detectable only by near-field techniques. This multi-technique approach offers a powerful framework for optimizing doping strategies in Sb_2Se_3 and related photovoltaic materials.

Keywords: TERS, Thin films, Photovoltaic, C-AFM, KPFM, doping

[Abstract:0062] [SERS/TERS/Plasmonics]

Comparative Evaluation of SERS Substrates for Reliable G-Quadruplex Detection

***Petra Petrović Popović*[1], *Tea Juračić*[1], *Nikša Krstulović*[2], *Snezana Miljanic*[1]**

[1]*Department of Chemistry, University of Zagreb Faculty of Science, Zagreb, Croatia*
[2]*Center for Advanced Laser Techniques, Institute of Physics, Zagreb, Croatia*

Surface-Enhanced Raman Scattering (SERS) spectroscopy is a powerful analytical tool for structural characterization of biomolecules. The quality, reproducibility, and interpretability of SERS spectra are strongly affected by the properties of the SERS substrates used in the experiment. This study presents a comparative evaluation of eight SERS substrates with respect to their performance in detecting conformational signatures of DNA G-quadruplexes.

Six colloidal suspensions of nanoparticles were synthesized by chemical reduction in solution, and two substrates were prepared by pulsed laser ablation in liquids. All substrates were comprehensively characterized by pH measurements, UV/Vis/NIR spectroscopy, scanning electron microscopy (SEM), dynamic light scattering (DLS), and zeta potential measurements. These parameters were used to establish differences in nanoparticle size, morphology, surface charge, aggregation behavior, and surface chemistry, providing a comprehensive basis for correlating substrate properties with SERS performance.

The human telomeric sequence Tel24 was used as a model system. SERS spectra were recorded for both its unfolded form and the antiparallel G-quadruplex conformation induced by high sodium ion concentrations. Comparative analysis focused on relative intensity ratios of characteristic adenine and guanine vibrational bands, which serve as structural markers for G-quadruplex folding.

Substrate performance was assessed based on the clear and reproducible detection of structure-sensitive adenine and guanine vibrational bands associated with Tel24 folding. The analysis included evaluation of relative intensity ratios of these marker bands, overall spectral clarity, background contribution, and consistency of spectral features. Differences among substrates were examined with respect to their suitability for reliable structural interpretation of unfolded and G-quadruplex conformations.

Based on the performed evaluation, citrate-stabilized silver nanoparticle colloids provided the most consistent and interpretable SERS spectra of Tel24. This work emphasized the importance of substrate selection and comprehensive physicochemical characterization for generating meaningful and reproducible SERS data in biomolecular studies. This comparative analysis provides practical insights for researchers applying SERS spectroscopy to complex nucleic acid systems.

Keywords: SERS, G-Quadruplex, Nanoparticles, Tel24, Raman Spectroscopy

[Abstract:0063] [Materials]

Vibrational Studies of Phase Transitions in Multilayered Hybrid Lead Halide Perovskites

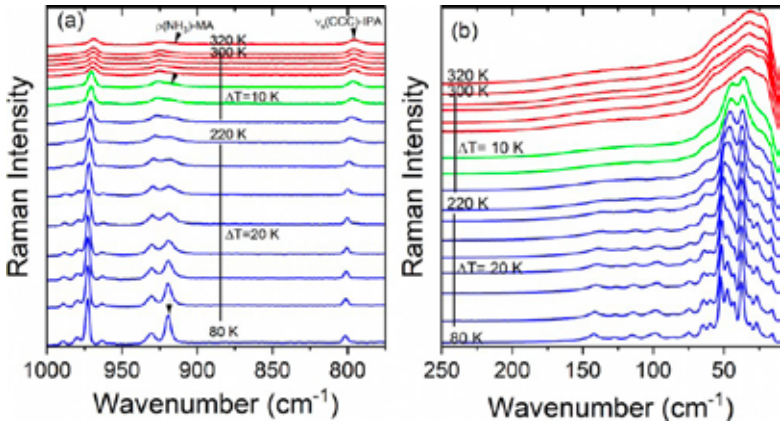
***Mirosław Mączka*, Szymon Smółka, Maciej Ptak**

Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okólna 2, 50-422, Wrocław, Poland

Hybrid organic-inorganic lead halide perovskites have attracted great interest in recent years due to their excellent optoelectronic properties that make them attractive for solar-cell, light-emitting, nonlinear optical, switchable dielectric and ferroelectric applications. One of such emerging group of perovskites are multilayered (n ≥ 2) Dion–Jacobson (DJ) (A"An1PbnX3n+1) and Ruddlesden–Popper (RP) (A'2An-1PbnX3n+1) compounds (A, A', A" and X denote small perovskitizer, large monovalent interlayer, large divalent interlayer cation, and halide anion, respectively). These compounds often undergo structural phase transitions associated with ordering of organic cations. Slowing down or freezing of the organic cation dynamics offers a way for inducing properties important for technological applications, such as ferroelectricity and second-order NLO properties. Due to complexity of these systems and twinning, it is often difficult to obtain structural information on the low-temperature polymorphs, and thus understand mechanism of the phase transitions and origin of functional properties based on X-ray diffraction data. Therefore, to obtain a full picture of structural, optical, and electric properties of multilayered perovskites, it is important to perform temperature-dependent studies of their phonon properties and dynamics of organic cations. We will show that temperature-dependent Raman and IR studies of DJ and RP multilayered perovskites comprising 1,4-butanediammonium (BDA2+) and isopropylammonium IPA+) cations, respectively, provide deep insight into mechanism of their phase transitions. Most importantly, vibrational spectroscopy allows to monitor the dynamics of perovskitizer and interlayer cations independently, allowing us to conclude that the higher temperature phase transition in IPA2MA2Pb3Br10 are triggered by ordering of MA+ cations (MA=methylammonium) while the second transition, observed at lower temperatures, is associated with ordering of IPA+ cations (Fig. 1a). Furthermore, Raman and IR methods provide information on the change in the organic cation conformation and distortion of the inorganic layers. As an example, we will discuss results obtained for a few BDA2+-based perovskites, which show that some of the phase transitions are associated with very pronounced change of the BDA2+ conformation, and IPA2MA2Pb3Br10, for which strong changes in the lattice mode region indicate pronounced effect of the phase transition on PbBr6 tilts and distortion (Fig. 1b).

Keywords: hybrid organic-inorganic perovskites, lead halides, Raman, infrared, phase transition

Figure 1



Raman spectra of IPA2MA2Pb3Br10 in the (a) 1000-775 cm-1 and (b) 250-10 cm-1 range

[Abstract:0064] [SERS/TERS/Plasmonics]

Nanoplastics Detection in Complex Cellular Environments by Tip-Enhanced Raman Spectroscopy

***Anushree Dutta*[1], *Stephan Handshin*[2], *Naresh Kumar*[1], *Renato Zenobi*[1]**

[1]*Department of Chemistry and Applied Biosciences, ETH Zurich, 8093 Zurich, Switzerland*
[2]*Department of Materials, ETH Zurich, 8093, Zurich, Switzerland*

Nanoplastics are emerging environmental contaminants with potential implications for human health; however, their trace-level detection and intracellular fate remain poorly understood. Conventional Raman spectroscopy enables non-destructive chemical identification of polymeric materials, yet its diffraction-limited spatial resolution restricts nanoscale localisation of nanoplastics within complex biological environments.[Nano Letters, 2023, 23(8), 3939–3946]

Here, we employ atomic force microscopy (AFM) combined with tip-enhanced Raman spectroscopy (TERS) for label-free nanoscale visualisation and chemical identification of polystyrene (PS) and polyvinyl chloride (PVC) nanoplastics in MCF10A human mammary epithelial cells. By combining the molecular specificity of Raman spectroscopy with the nanometre-scale spatial resolution provided by a scanning probe metallic tip, TERS enables direct chemical fingerprinting of individual nanoplastic particles within complex cellular environments. Transmission electron microscopy and confocal imaging studies reveal that PS nanoplastics predominantly localise within endosomal compartments, indicating uptake through endocytic pathways. In contrast, PVC nanoplastics exhibit a more dispersed distribution and form vesicle-like structures in the cytoplasm that are spatially distinct from endo-lysosomal regions, revealing polymer-dependent intracellular behaviour. Cytotoxicity measurements further show a significantly higher cellular stress response for PVC exposure (~40%) compared to PS (~10%), indicating that polymer-dependent localisation and intracellular interactions may influence cellular toxicity. [Particle and Fibre Toxicology, 2012, 9, 20]

Therefore, TERS enables direct nanoscale chemical identification of nanoplastic particles, demonstrating the power of label-free nanospectroscopy for probing environmental nanomaterials in biological systems.

Keywords: Plastic Pollution, Tip-enhanced Raman Spectroscopy, Nanoplastics, Cellular Detection, Single Particle Spectroscopy

[Abstract:0065] [Biology/Biomedicine]

Multimodal Spectroscopic Evidence of Selective Cytotoxic and Radiosensitizing Effects of Withaferin a İn Cervical Cancer Cells

***Ewa Pięta*, Agnieszka Panek, Monika Szczepanek-Dulska, Katarzyna Pogoda**

Institute of Nuclear Physics Polish Academy of Sciences, PL-31342, Krakow, Poland

Cervical cancer therapy remains limited by insufficient tumor selectivity and plateauing cytotoxic responses to moderate radiation doses. This study investigates the anticancer and radiosensitizing potential of withaferin A (WFA), a vimentin-targeting adaptogenic compound, in primary and metastatic cervical cancer models using an integrated multimodal analytical approach (Figure 1) [1,2].

WFA induced a dose-dependent reduction in cell viability, with primary C-33A cells exhibiting markedly greater sensitivity than metastatic CaSki cells and non-cancerous fibroblasts. Flow cytometric analysis demonstrated that at a concentration of 2 μM WFA, more than 90% of C-33 A cells underwent late apoptosis, compared with approximately 18% of CaSki cells and 10% of fibroblasts, confirming pronounced tumor selectivity. Comet assay revealed significantly elevated DNA strand breaks in cancer cells, particularly in C-33 A, whereas normal fibroblasts showed minimal genotoxic response. Fluorescence imaging and AFM topography analysis demonstrated cytoskeletal disorganization, reduced cellular and nuclear areas, and membrane alterations consistent with apoptotic progression. Molecular docking supported the feasibility of non-covalent interactions between WFA and vimentin, providing a structural rationale for cytoskeletal destabilization.

Baseline irradiation experiments revealed a plateau of cytotoxic response above 1–2 Gy in cervical cancer cells, underscoring the need for radiosensitizing strategies. Notably, WFA significantly potentiated the effects of 1 Gy irradiation, enhancing both cytotoxicity and DNA damage. Metastatic CaSki cells, relatively resistant to WFA alone, exhibited pronounced genotoxic and cytotoxic responses under combined treatment, indicating a predominantly radiosensitizing mechanism [2].

Single-cell FT-IR and Raman spectroscopic imaging coupled with chemometric analysis revealed extensive molecular remodeling following WFA exposure and combined treatment. Dominant alterations involved protein secondary structure, lipid membrane composition, and nucleic acid–associated bands. In selected models, Raman signatures associated with mitochondrial cytochromes suggested activation of mitochondrial-mediated apoptotic pathways, whereas other phenotypes displayed membrane-associated spectral changes, reflecting cell-line–dependent mechanisms of response.

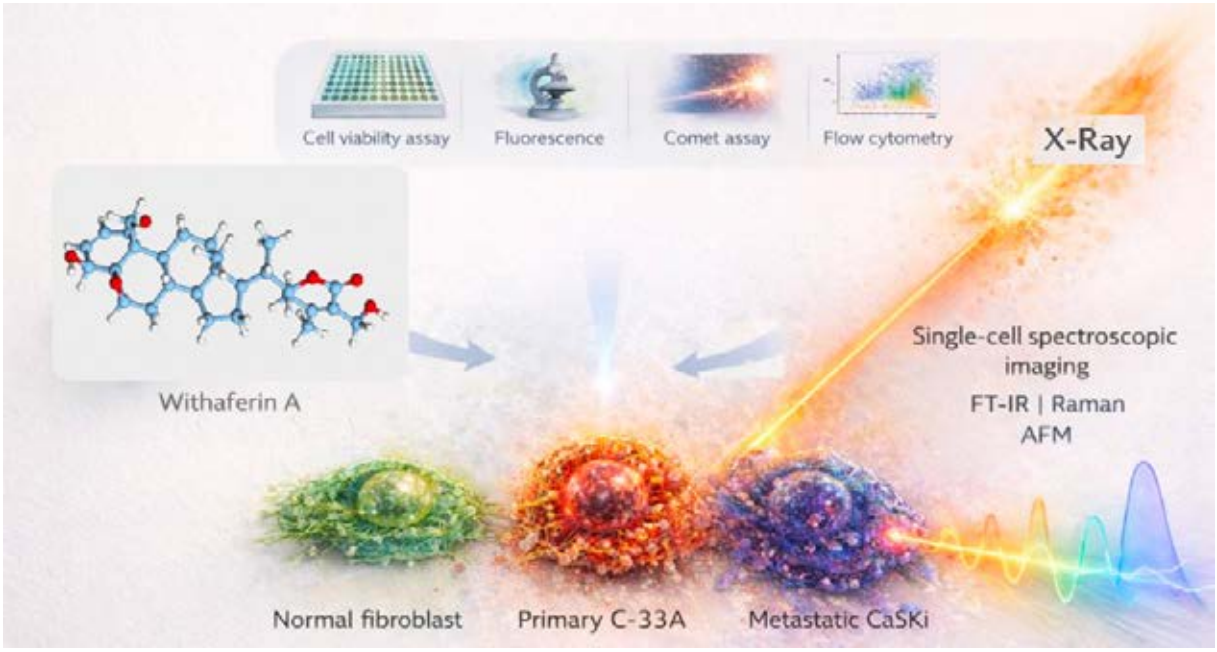
References:

[1] E. Pięta, A. Panek, M. Szczepanek-Dulska, K. Pogoda, Vimentin-targeting adaptogen withaferin A: Potential to selectively suppress cervical cancer – Single-cell microspectroscopic and molecular analysis, BBA – Mol. Basis Dis. 1872 (2026) 168125.

[2] E. Pięta, A. Panek, K. Pogoda, Radiosensitizing potential of withaferin A in cervical cancer cells revealed by multimodal spectroscopic imaging, submitted for publication.

Keywords: adaptogen, cervical cancer cells, withaferin A, single-cell spectroscopic imaging, vimentin, radiosensitization

Figure 1. Schematic illustration of the experimental workflow and cellular response to withaferin A and X-ray irradiation in cervical cancer models.



[Abstract:0067] [Novel Approaches]

The Structure of Raman Excitation Maps From Pure Carbon Nanotube Materials

***Paul Finnie*[1], *Adam Wind*[2], *Jianying Ouyang*[1], *Jeffrey A. Fagan*[3]**

[1]*Quantum and Nanotechnologies Research Centre, National Research Council Canada, 1200 Montreal Road, Ottawa, Ontario, K1A 0R6, Canada*
[2]*University of Waterloo, 200 University Avenue West, Waterloo, ON, N2L 3G1, Canada*
[3]*Materials Science and Engineering Division, National Institute of Standards and Technology (NIST), Gaithersburg, Maryland, 20899, United States*

Here we use a resonant excitation mapping (REM) technique to obtain the Raman scattering (RS) spectra and their excitation profiles from thin films samples of chirality pure single walled carbon nanotubes (SWCNTs) in real time. We have been developing a rapid technique to obtain REM - the RS spectra and optical excitation spectra together.[1] RS is one of the most well-developed characterization tools for nanocarbons. RS from SWCNT materials is typically resonant, making today's chirality-pure SWCNT materials ideal to investigate. We investigate several different chiralities and preparation methods.

REMs encode details about both electronic and vibrational properties, so they are even more information-rich than RS spectra alone. We have extended REM over a broad range of incident photon energies [2], with excitation covering the visible and extending into the near infrared. This allows us to sensitively track the evolution of bands in real time, for example as they change due to the accumulation of photo-induced defects.[3] We explore not just phonon emission, as is most common, but also phonon absorption (Anti-Stokes RS)[4]. As we can see many bands and their excitation spectra simultaneously, this is a good experimental test of the form of the Raman scattering matrix element. In general, even simple electronic structures give rise to intricate structures in the REM, which we trace out experimentally and connect to simple theory. We believe REM like this has great potential for SWCNT material characterization, metrology and fundamentals, and more generally for any kind of sample showing resonant RS features.

References:

[1] Finnie P, Ouyang J, Lefebvre J, Full Spectrum Raman Excitation Mapping Spectroscopy, Sci. Rep. (2020); 10, 9172

[2] Finnie P, Ouyang J, Fagan JA, Broadband Full-Spectrum Raman Excitation Mapping Reveals Intricate Optoelectronic–Vibrational Resonance Structure of Chirality-Pure Single-Walled Carbon Nanotubes, ACS Nano (2023); 17, 7285

[3] Finnie P, Ouyang J, Fagan JA, Static and Dynamic Raman Excitation Mapping of Chirality-Pure Carbon Nanotube Films, Comm. Mat. (2025); 6, 10

[4] Finnie P, Wind A, Ouyang, J., Shapturenka P., Fagan JA, The Resonance Structure of Raman Scattering for Emitted and Absorbed Phonons in Chirality-Pure Carbon Nanotube Films, ACS Nano (2025); 19, 39793

Keywords: Raman excitation map, Raman excitation profile, resonant Raman spectroscopy, carbon nanotube, nanocarbon

[Abstract:0071] [Novel Approaches]

Rapid Microplastic Imaging Enabled by a Pulsed UV Raman Microscope

***Felix Schröter*, Dávid Jenő Palásti, Jens Riedel**

Federal Institute for Materials Research and Testing (BAM), Berlin, Germany

Today's omnipresence of microplastic particles poses an imminent threat to the environment and health. Consequently, many analytical techniques have been suggested for their detection and identification regarding size and chemical composition. Among these, Raman microspectroscopy combines chemical identification of polymers with micrometer spatial resolution, but its conventional visible-light excitation requires long integration times, impractical for mapping experiments with sufficient throughput. Extensive and high-resolution mapping can thus extend measurement times to several days.

We present a highly accelerated UV-Raman microscope based on the 355 nm output of a DPSS laser for excitation to overcome long measurement times and to take advantage of the benefits UV excitation offers. UV light exhibits enhanced Raman scattering which makes drastically shorter integration times viable, leading to an overall reduction in measurement times. Furthermore, UV Raman can be conducted in ambient light, thus simplifying integration into processes and workflows. Additionally, UV light allows for tighter focusing and therefore good spatial resolution can be realized even with cost-effective optics, allowing for a rapid and low-cost setup.

The presented microscope was able to extensively map 256 mm^2 of dispersed microplastic particles in under eight hours. The analyzed microplastics consisted of four cryo-milled end of life polymer products distributed across a silicon wafer. An integration time of only 100 ms led to the collection of more than 140,000 spectra in this period allowing for the identification and mapping of microplastics. For the unambiguous identification of polymers with sufficient discrimination within the resulting large dataset unsupervised classification algorithms were successfully employed. As a result, combining fast UV-Raman and unsupervised classification schemes, mapping and classification can be achieved within a single working day.

Keywords: UV Raman Microspectroscopy, Microplastics, Instrumentation

[Abstract:0073] [Biology/Biomedicine]

Raman Spectroscopy for Bacterial Identification: From Full Cultivation to In Vivo Measurements

***Lucía Ronda*[1], *Danylo Komisar*[1], *Andrii Kutsyk*[1], *Ditte Rask*[2], *Thomas Emil Andersen*[2], *Gohar Soufi*[3], *Oleksii Ilchenko*[1]**

[1]*Lightnovo ApS, Blokken 11, 1., Birkerød, Denmark*
[2]*Department of Clinical Microbiology, Odense University Hospital, 5000 Odense, Denmark*
[3]*Technical University of Denmark, 2800 Lyngby, Denmark*

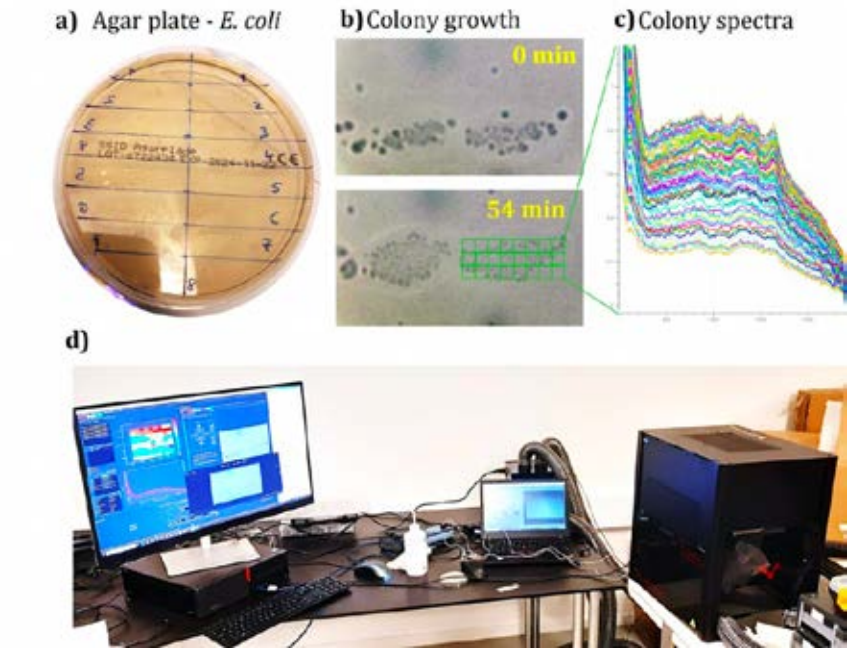
We present a comparison of machine learning (ML) based Raman spectroscopy for bacterial identification across three approaches: after full cultivation, after fast cultivation, and in vivo, evaluating their accuracy and limitations.

The rapid and accurate identification of bacterial pathogens remains a critical challenge in clinical diagnostics, where delays in targeted treatment may lead to poor patient outcomes and the empirical administration of antibiotics. Currently, the gold standard for bacterial identification is MALDI-TOF mass spectrometry (MS). While the identification step itself is relatively fast (~30 minutes), the technique requires a mandatory pre-cultivation period of approximately 24 hours and specialized laboratory infrastructure. Furthermore, discrimination between closely related strains may remain challenging [Microbiol. Spectr. 2025, 13, 3, e01425–24]. In this work, we investigate Raman spectroscopy combined with Machine Learning (ML) as a faster, cost-effective alternative for bacterial identification [Nat. Commun. 2019, 10, 1, 4927].

We evaluate a progressive transition from conventional full cultivation protocols to fast cultivation conditions (Figure 1) and ultimately to in vivo measurements, where Raman spectra are acquired directly from chronic wounds in a clinical setup. We aim to investigate the robustness of spectral classification under biologically complex and heterogeneous conditions. Raman spectra are analyzed using multivariate and machine learning–based methods to differentiate bacterial species. Results are benchmarked against MALDI-TOF MS to evaluate agreement and diagnostic performance. Preliminary results from 5-fold cross-validation with 10 repetitions yielded a prediction accuracy of 0.9651 ± 0.0095 (Figure 2), the capability to distinguish pathogens directly from patient-derived samples. These findings support Raman spectroscopy as a promising optical approach for accelerating pathogen identification.

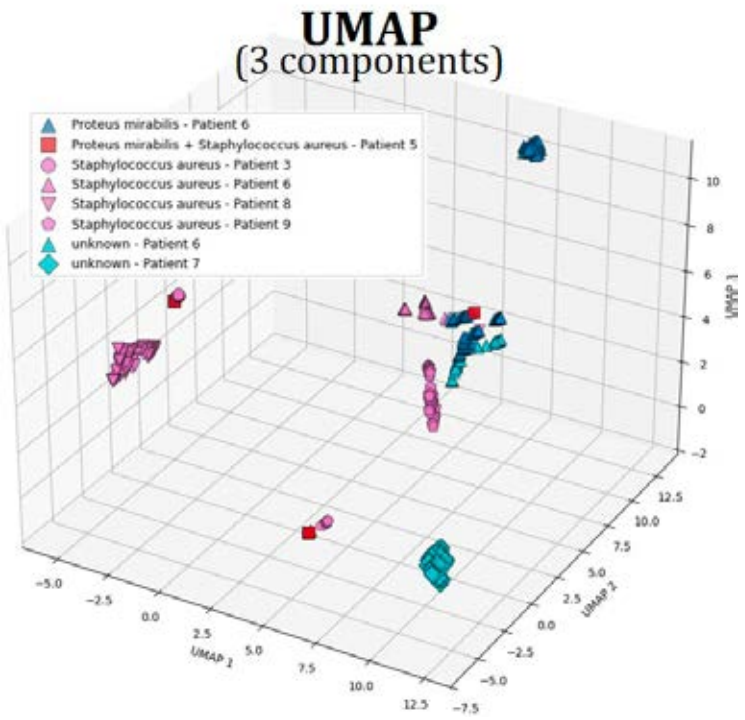
Keywords: Raman Spectroscopy, Machine Learning, Bacteria Identification, MALDI-TOF, Mass Spectrometry

Figure 1: Measurement workflow under fast cultivation conditions



(a) Bacteria are placed on an agar plate, (b) colony growth for 1 hour at 37°C, (c) Raman spectral acquisition, and (d) experimental setup including the Lightnovo microscope and analysis system

Figure 2: Preliminary classification results obtained without cultivation



Raman spectra differentiate Proteus mirabilis (dark blue), Staphylococcus aureus (pink), their combination (red), unknown (light blue). Marker shape indicates patient origin; some patients present multiple bacterial types

[Abstract:0074] [Biology/Biomedicine]

Label-Free Evaluation of Drug Effects in Brain Organoids and Spheroids Using Raman Spectroscopy

***Giulia Bruno*[1], *Naja Burgers*[2], *Eike Collen*[2], *Andrea Giovanale*[1], *Julien Hurtaud*[1], *Michele Dipalo*[1], *Marcel Leist*[2], *Francesco De Angelis*[1]**

[1]*Italian Institute of Technology*
[2]*University of Konstanz*

Three-dimensional neural models such as brain organoids and spheroids are increasingly used for preclinical drug testing because they better reproduce the biochemical and structural complexity of neural tissue compared to traditional two-dimensional cultures. However, most analytical methods used to assess drug responses rely on destructive assays, preventing longitudinal monitoring of the same sample and limiting the ability to capture dynamic biochemical changes during treatment.

Here, we present a label-free approach based on Raman Spectroscopy (RS) combined with multivariate analysis and machine learning to evaluate drug effects in brain organoids and spheroids. Principal Component Analysis (PCA) was first used to reduce spectral dimensionality and extract latent variables capturing the main sources of biochemical variability. The resulting PCA space was further explored using classification methods, including Random Forest (RF) and Linear Discriminant Analysis (LDA) applied to PCA scores, enabling discrimination between treated and untreated samples and highlighting spectral patterns associated with drug exposure.

Importantly, the non-invasive nature of RS enables repeated measurements of the same organoids and spheroids over time, allowing longitudinal tracking of drug-induced biochemical changes. These results highlight the potential of RS as a high-content, label-free tool for dynamic drug evaluation in complex neural 3D models and for future applications in preclinical screening.

Keywords: Raman Spectroscopy, Organoids, Drug screening, Machine Learning

[Abstract:0075] [SERS/TERS/Plasmonics]

Two-Dimensional Thiophosphites Enhanced Raman Scattering: From Sub-Zeptomolar Sensing to SixteenOrder-of-Magnitude Quantitative Analysis

Wenjun Chen

School of Electronic Information Engineering, Guangdong Provincial Key Laboratory of Industrial Intelligent Inspection Technology, Foshan University, Foshan, P. R. China

Quantum sensing with ultrahigh sensitivity to external environment has shown advantages over its classical counterparts, driving significant progress of the nanoscience and nanotechnology. Among the advanced techniques, plasmon-free surface-enhanced Raman scattering (SERS) has drawn intensive research attention largely due to its single-molecule detection of limit (LOD), high biocompability, and high stability. In recent, SERS platforms are required not only to detect molecules but also to quantify them at the ultralow concentration. Herein, we introduce a mechanochemical strategy [*Nat. Commun.* 2024, *15*, 10195], which combines the wrinkling and chemical functionalization, to fabricate a plasmon-free SERS platform based on two-dimensional (2D) MnPS3 with a sub-zeptomolar (10^{-22} M) LOD and an ultrahigh enhancement factor of 1.30×10^{12} (Figure 1). This mechanism is clarified that the construction of wrinkles in 2D MnPS3, which serve as active boundaries to improve the light-matter coupling, as well as the SERS performance. In addition, the amino groups in primary amine molecules decorated on 2D MnPS3 surface are crosslinkers that create more pathways to promote charge transfer between these substances. On this basis, we propose a signal-squeezing strategy for quantitative detection of analytes in a concentration range spanning 16 orders of magnitude, using four distinct plasmon-free SERS platforms for the first time (Figure 2). Each platform is engineered to be optimally sensitive to a specific and continuous concentration window, collectively covering 10^{-6} to 10^{-22} M. For each platform, raw spectral characteristics are transformed into a vector (intensity, signal-to-noise ratio, probability) that four tri-parametric radar maps of the concentration windows were created as the calibration charts, respectively. To quantify a solution with an unknown concentration, its experimental tri-parametric vector is projected onto this set of radar charts. The triangular area bounded by lines connecting the vector points is 'squeezed' by two adjacent regions, which provides the readout of the solution's concentration level. This work broadens the use of 2D materials in quantum sensing technology, but also provides a solution to advance the SERS technique as the mainstream tool in biosensing, food safety, and environmental surveillance.

Keywords: surface-enhanced Raman scattering, 2D materials, quantitative detection, light-matter interaction, charge transfer

Figure 1. Mechanochemical concept for designing SERS platform and its sensing performance.

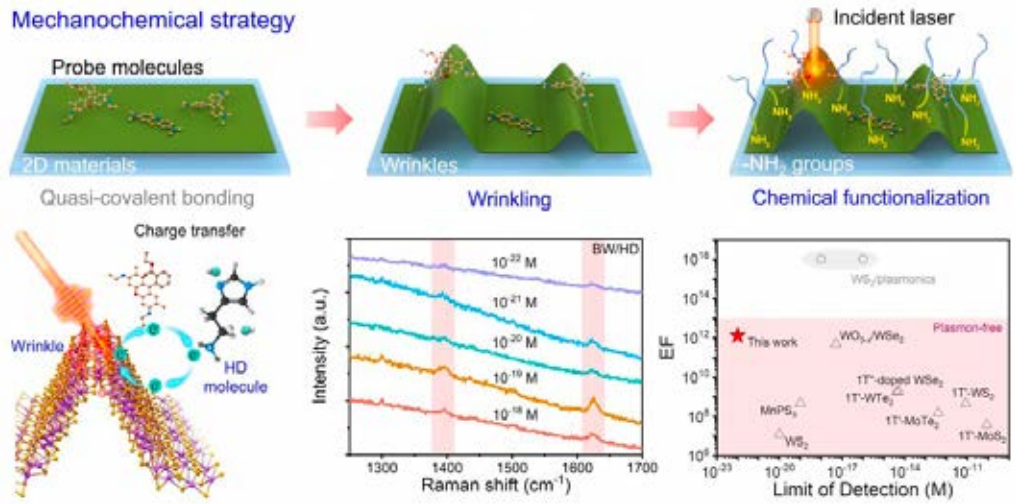
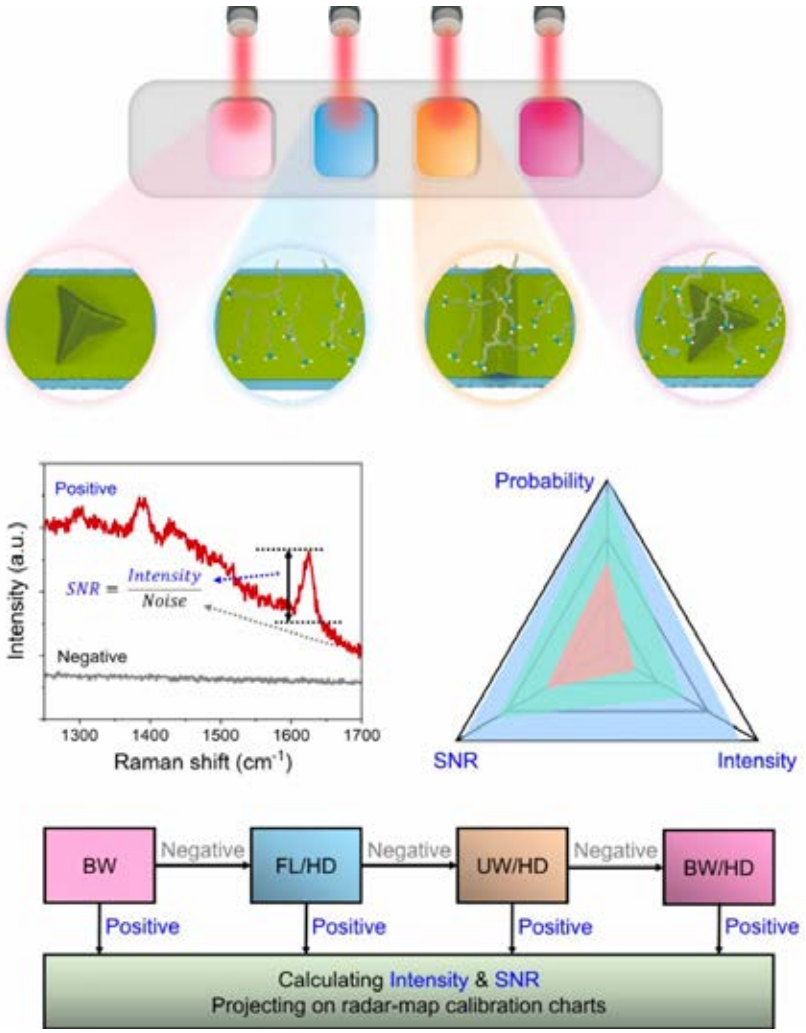


Figure 2. Signal-squeezing strategy for quantitative analysis of molecules based on SERS spectroscopy.



Oral Abstracts

[Abstract:0077] [Novel Approaches]

High-Speed AFM/micro-Raman Multimodal Measurement System: Correlative Analysis of Conformational and Chemical-Bond Dynamics

***Keishi Yang*[1], *FengYueh Chan*[2], *Takayuki Uchihashi*[2], *Prabhat Verma*[1], *Takayuki Umakoshi*[1]**

[1]*Applied Physics, The University of Osaka, Osaka, Japan*
[2]*Physics, Nagoya University, Aichi, Japan*

High-speed atomic force microscopy (HS-AFM) is a powerful tool for observing the conformational changes of living biomolecules as real-time movies due to its high spatial (~1 nm) and temporal resolution (<10 frames per second) through rapid cantilever scanning [*Proc. Nat, Acad. Sci. U. S. A.* 2001, 98, 12468]. Moreover, by analyzing not only conformational changes but also the underlying chemical dynamics, more detailed mechanisms of biomolecular functions can be revealed. By combining HS-AFM with Raman spectroscopy, one can study both conformational changes and chemical-bond dynamics simultaneously, which drastically enhances the analytical capability for elucidating complex biological phenomena.

In this study, we developed an HS-AFM/micro-Raman multimodal system for correlative nanoscale analysis of conformational and chemical-bond dynamics (Figure 1(a)). A stand-alone tip-scanning HS-AFM was employed [*Rev. Sci. Instrum.* 2013, 84, 073706], which is suitable for integration with an optical setup [K. Yang et al., *Nano Lett.* 2024, 24, 2805]. We integrated a Raman optical setup which can align the focal position of the excitation laser for Raman measurements with the HS-AFM observation area precisely. This setup ensures that topographical images and Raman spectra are collected from the same region simultaneously. Both the observation area of HS-AFM and the laser focal size for Raman measurement are several hundred nm, which allows the detection of Raman spectra from the area observed by HS-AFM. This system synchronizes the two measurements to acquire one Raman spectrum per HS-AFM image frame, facilitating correlative analysis of structural and chemical changes. Using this system, we successfully demonstrated HS-AFM/Raman multimodal measurements of 2D materials flakes of graphene and MoS2. Characteristic Raman spectra were detected exclusively when the respective materials were present within the HS-AFM observation area, which confirmed this system successfully correlated topographical images with chemical analysis (Figure 1(b)). We will also demonstrate several HS-AFM/micro-Raman multimodal observations using various samples.

Keywords: spontaneous Raman, high-speed AFM, AFM-Raman

Figure 1

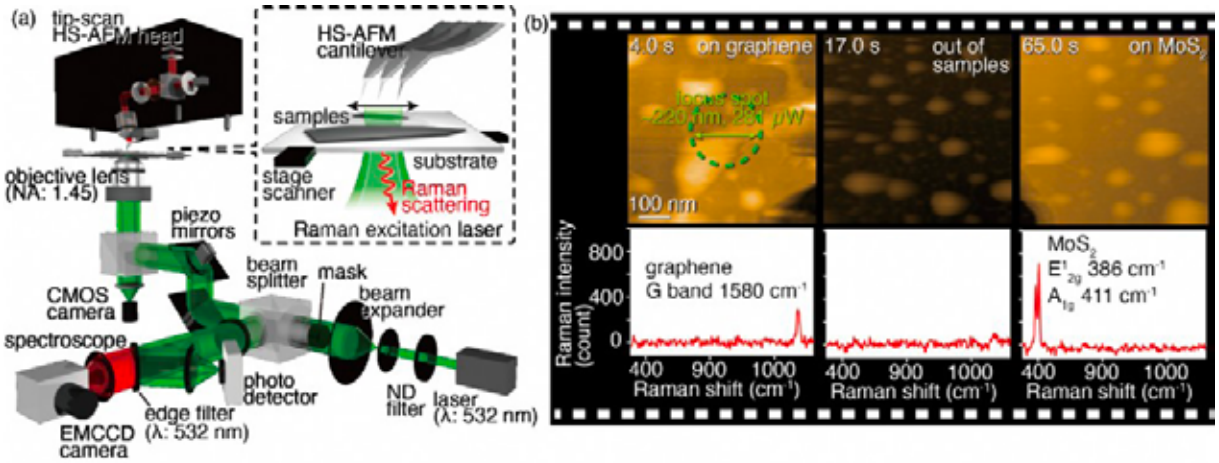


Figure 1. (a)Schematic image of HS-AFM/micro-Raman multimodal system (b)HS-AFM/micro-Raman image of 2D materials

[Abstract:0079] [Biology/Biomedicine]

Minimally Invasive Raman Spectroscopy: Applications for Oral Cancer Assessment

***Murali Krishna Chilakapati*, Panchali Saha, Arti Hole, Vikram Gota, Pankaj Chaturvedi, Poonam Joshi**

Tata Memorial Centre, Advanced Centre for Treatment, Education and Research in Cancer, Kharghar Navi Mumbai, Maharashtra, India

A large and steadily increasing number of oral cancer cases are reported worldwide each year, highlighting its growing global health burden. Early diagnosis of oral cancer is essential for improving patient survival rates. Despite advances in therapeutic modalities, mortality rates remain high as cases are often presented in late stages. Reliable screening tools for high-risk populations in necessary. The invasive nature of the gold standard detection method, biopsy, limits its suitability for large-scale screening. Raman spectroscopy of biological samples has emerged as a promising and minimally invasive technique capable of capturing biochemical alterations associated with malignant transformation. Distinguishing malignant conditions from non-diseased states remains challenging, particularly in individuals without clinically evident lesions, due to field cancerization and subclinical molecular changes. These challenges highlight the need for improved risk stratification strategies that can support early detection. In this study, Raman spectroscopy was applied to minimally invasive specimen like –blood serum, urine and saliva from oral cancer patients and control subjects. Spectral data were acquired with WITec 300R alpha confocal Raman instrument with a 532 nm excitation laser, followed by preprocessing and multivariate analysis to build classification models. The supervised classification models demonstrated good precision for the identification of control cases, and reliably identified malignant cases, though varied across the specimen with sera showing better classification. These findings support the potential of Raman spectroscopy as a minimally invasive modality for rapid screening of high-risk cases.

Keywords: Raman spectroscopy, Oral cancers, minimally invasive

[Abstract:0085] [Biology/Biomedicine]

Stage-Dependent Mechanisms of Action of Antimalarial Drugs on Hemozoin Formation in Infected Erythrocytes

***Timea Frosch*[1], *Juergen Popp*[1], *Torsten Frosch*[2]**

[1]*Spectroscopy and Imaging Department, Leibniz-Institute of Photonic Technology, Albert-Einstein-Str.9, 07745, Jena, Germany*
[2]*Biophotonics and Biomedical Engineering, Technical University Darmstadt, Rundeturmstrasse 12, 64283, Darmstadt, Germany*

Malaria, caused by *Plasmodium spp*. parasite, remains a major global health challenge, particularly in sub-Saharan Africa, necessitating innovative strategies to meet the WHO target of a 90% reduction in incidence and mortality by 2030 [WHO: World Malaria Report, 2025]. Achieving this goal requires improved prevention, surveillance, and therapeutic approaches, supported by detailed molecular-level understanding of drug–target interactions within infected cells to overcome emerging drug resistance. Hemozoin biocrystallization constitutes a key detoxification pathway in *Plasmodium falciparum* and represents a principal molecular target of antimalarial drugs. Direct *in situ* spectroscopic characterization of drug–hemozoin interactions within infected red blood cells (iRBCs), particularly with parasite stage resolution, remains limited.

Here, resonance Raman microspectroscopy is employed to investigate drug-induced perturbations of hemozoin formation directly under intracellular conditions [Timea Frosch et al., *Stage-Dependent Mechanisms of Action of Antimalarials - Focused on Hemozoin Formation in Infected Erythrocytes*, submitted]. Stage-resolved Raman measurements (λexc = 647 nm) were performed on *P. falciparum*–infected erythrocytes treated with chloroquine (CQ), artemether (ARTE), and the trioxaquine hybrid DU1302 (TQ). Resonance enhancement enabled selective probing of porphyrin vibrational modes sensitive to hemozoin crystallinity and structural modification directly within intact cells. Comparative spectral analysis reveals distinct drug- and stage-dependent effects associated with differences in pharmacophore architecture.

CQ and ARTE predominantly interfere with early hemozoin nucleation during the ring stage, reflected by systematic changes in characteristic porphyrin marker bands. In contrast, TQ primarily affects crystal growth during the trophozoite stage. Additional spectral signatures indicate *in situ* alkylation of hemozoin by ARTE and TQ. Density functional theory (DFT) calculations support assignment of observed spectral changes and suggest a preferential formation as δ-isomer for the ARTE–hemozoin alkylated complex.

These results provide spectroscopic evidence of stage-dependent drug action and demonstrate the capability of resonance Raman microspectroscopy for non-destructive investigation of intracellular drug–target interactions. Beyond elucidating mechanisms of antimalarial action, the presented approach highlights the potential of Raman-based methodologies for *in situ* pharmacodynamic studies as well as understanding and thus controlling novel therapeutic approaches like cell therapies.

Keywords: in situ drug-target analysis, Resonance Raman Microspectroscopy, antimalarials, iRBCs

Oral Abstracts

[Abstract:0087] [Novel Approaches]

Gemstones and Minerals Identification Using Machine Learning Assisted Raman Spectroscopy

***Yaroslav Aulin*[1], *Andrii Kutsyk*[1], *James Thomson*[2], *Christian Charriere*[3], *Danylo Komisar*[1], *Georgios Apostolou*[4], *Konstantinos Stergiou*[1], *Yurii Pilhun*[1], *Oleksii Ilchenko*[1]**

[1]*Lightnovo ApS, Birkerod, Denmark*
[2]*Lightnovo UK, Harmodsworth, UK*
[3]*Gem Swiss Stone Factory, Montreux, Switzerland*
[4]*Department of Physics, Technical University of Denmark, Lyngby, Denmark*

We present a high-accuracy, machine learning-based methodology for gemstone classification using Raman spectroscopy. Raman spectra were collected across multiple points per sample using a 785 nm excitation source, followed by outlier rejection to eliminate fluorescence-dominated data. Dimensionality reduction via principal component analysis (PCA) was applied prior to classification using several machine learning models. Among the models tested, the Random Forest algorithm achieved the highest accuracy of 95.6%, significantly outperforming conventional Pearson correlation-based spectral matching (50.6%). The approach was validated across 96 different gemstone and minerals classes including fine distinctions within closely related mineral families such as quartz, beryl, and corundum.

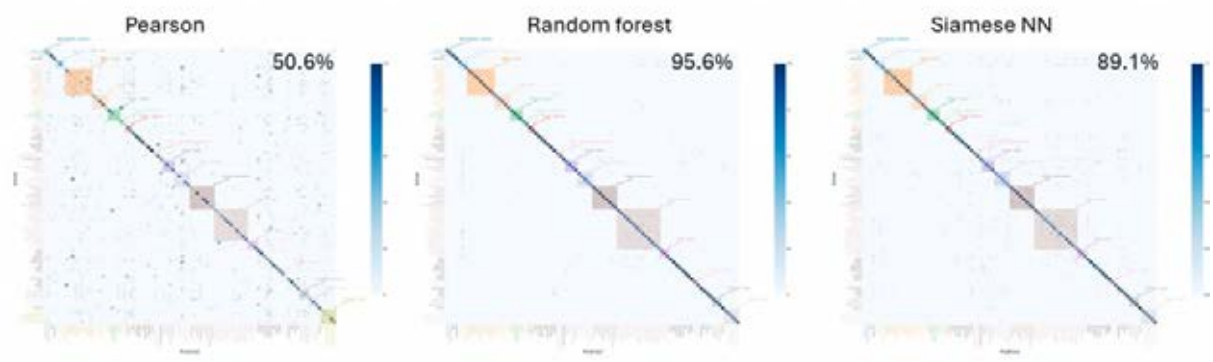
Additionally, we explore the neural network approach, Siamese neural networks in particular. Such an approach allows for easy expansion of the model with new classes without need for retraining as well as implementation of data augmentation during training in order to build more robust classification models. The performance of the Siamese model in terms of accuracy is currently slightly worse (89.1%) than that one of the random forest model (95.6%), however we find the Siamese model the most promising approach due to the above-mentioned advantages such as robustness and scalability what is expected to lead to the best real-world performance of the model when deployed.

Figure 1. Normalized confusion matrix for Pearson library search (left) versus Random Forest algorithm (center) versus Siamese neural network model (right). Diagonal components correspond to correct identifications while off-diagonal correspond to misidentifications. The minerals are grouped into families corresponding to the diagonal blocks in the confusion matrix.

We also perform the comparison of different excitation laser wavelengths: 405, 532, 638, 785, 830 nm. We show that the performance at 830 nm in terms of identification is the best, we attribute this to minimized fluorescence from the samples.

Keywords: Raman spectroscopy, identification, machnie learning, Siamese neural networks

ICORS_Aulin



[Abstract:0090] [Biology/Biomedicine]

Systematic Investigation of Drug Resistance Reversal in Triple Negative Breast Cancer Using Raman Spectroscopy

Zeynep Kilinc*, *Gamze Yesilay

Affiliation 1: University of Health Sciences, Experimental Medicine Application & Research Center, Validebag Research Park, 34662, Turkiye, Affiliation 2: Department of Molecular Biology and Genetics, University of Health Sciences, 34668, Turkiye

Gemcitabine-resistant triple-negative breast cancer (TNBC) remains a major clinical challenge driven in part by P-glycoprotein (P-gp)–mediated drug efflux. The study evaluates whether combined Berberine and Dactolisib treatment can modulate P-gp–associated resistance mechanisms in Gemcitabine-resistant TNBC cell lines, employing a multidisciplinary suite of biophysical and molecular assays including LigandTracer (a real-time binding kinetics evaluation instrument) and Raman spectroscopy coupled with complementary molecular biology techniques such as Western blotting, quantitative PCR, flow cytometry, and immunofluorescence to interrogate P-gp expression, membrane dynamics, and downstream signaling.

A standardized experimental pipeline was implemented to ensure reproducibility across resistant models. Orthogonal readouts combined kinetic binding profiles, nanoscale membrane mechanics, and molecular spectral fingerprints with targeted molecular assays and functional validation using an established P-gp inhibitor Zosuquidar and membrane dynamics probes. Experimental conditions were optimized to permit cross-validation between biophysical and biochemical endpoints.

Preliminary analyses across these complementary platforms consistently indicate modulation of P-gp-related activity and membrane biophysical properties following combined Berberine-Dactolisib exposure. Trends from spectral and molecular assays align with functional measures of efflux capacity, supporting the central hypothesis that the combination attenuates P-gp-mediated resistance phenotypes in Gemcitabine-resistant TNBC models. Outcomes demonstrate feasibility for producing standardized, high-content datasets suitable for translational data platforms and clinical decision support development.

Keywords: Drug Efflux, Cell Membrane Dynamics, Multidrug Resistance, Raman Spectroscopy, Berberine

Oral Abstracts

[Abstract:0091] [Biology/Biomedicine]

DTNR-SORS: A Hardware Solution to the Sensitivity Bottleneck in Raman Glucose Sensing

***Danylo Komisar*[1], *Khorshid Kamguyan*[2], *Andrii Kutsyk*[1], *Yurii Pilhun*[1], *Konstantinos Stergiou*[1], *Anja Boisen*[2], *Stefan Ovesen Banke*[3], *Oleksii Ilchenko*[1]**

[1]*Lightnovo ApS, Birkerød, Denmark*
[2]*Center for Intelligent Drug Delivery and Sensing Using Microcontainers and Nanomechanics (IDUN), Department of Health Technology, Technical University of Denmark, Kongens Lyngby, Denmark*
[3]*Department of Space Research and Space Technology, Technical University of Denmark, Kongens Lyngby, Denmark*

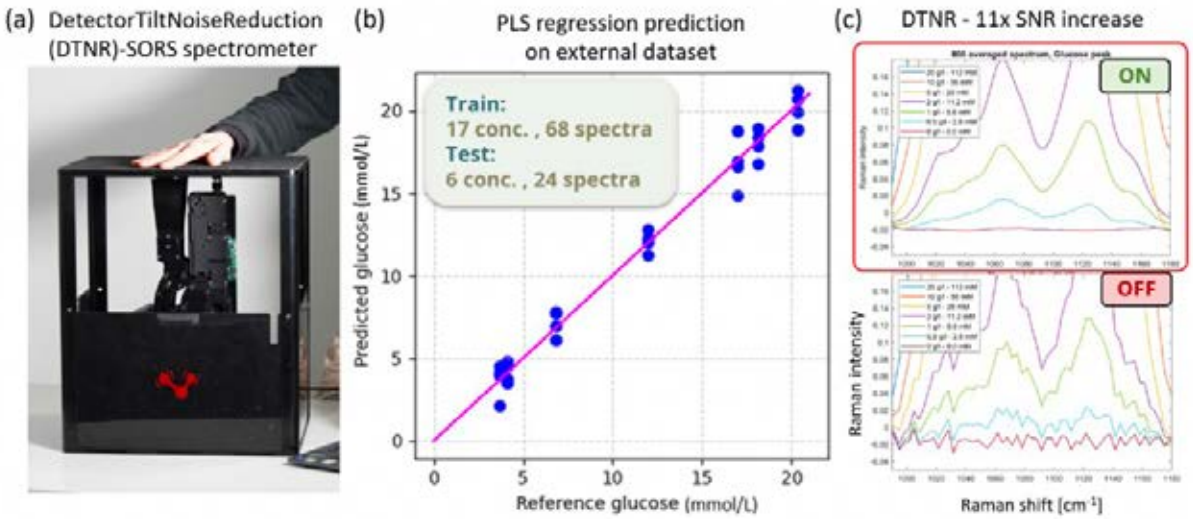
We present a Raman-based approach to non-invasive glucose monitoring that combines Spatially Offset Raman Spectroscopy (SORS) with Detector-Tilt Noise-Reduction (DTNR) technology. While Raman spectroscopy can already detect elevated glucose levels in tissue, reliable detection at clinically critical low concentrations remains a major challenge. Hypoglycemic conditions (<3 mmol/L) represent the most dangerous physiological range, yet Raman measurements often struggle precisely in this regime because the weak spectral signal approaches the detection limits of current instrumentation. Achieving sufficient signal-to-noise ratio (SNR) typically requires long acquisition times (>4 min), where detector-related noise and pixel sensitivity variations become significant.

The DTNR method directly addresses this limitation by compensating pixel-sensitivity variations in deep-cooled CCD detectors during long-exposure measurements, providing ~10× improvement in SNR. In combination with SORS, which enables depth-selective probing of interstitial fluid in the dermis while minimizing epidermal interference, this approach improves sensitivity for physiologically relevant glucose concentrations and addresses a key limitation reported in previous Raman glucose studies: insufficient sensitivity and reproducibility across patients.

We demonstrate prototype measurements and initial validation results from laboratory testing on a volunteer. A partial least squares (PLS) model was used to predict glucose concentration from multi-channel depth-resolved Raman spectra. The model was trained on a dataset of 17 glucose concentrations (68 spectra) and evaluated on 6 concentrations (24 spectra). Channels collecting Raman signals from 300–500 μm depth showed higher correlation with glucose concentration than surface channels. Beyond glucose sensing, the platform enables high-sensitivity non-invasive skin analysis for metabolic monitoring, dermatology, and pharmaceutical research.

Keywords: Raman, SORS, noise, glucose, skin

Non-invasive glucose monitoring proof-of-concept experiment.



Non-invasive glucose monitoring proof-of-concept experiment. (a) The prototype system. (b) PLS (partial least squares) model for glucose level prediction, comprising 17 concentrations/68 spectra in the training set and 6 concentrations/24 spectra in the external validation set. (c) Glucose peaks in water measured with and without Detector-Tilt Noise-Reduction. DTNR method eliminates pixel quantum-efficiency variation noise, achieving ~11× improvement in signal-to-noise ratio for low-concentration long-exposure measurements.

[Abstract:0092] [Coherent Raman Imaging]

Single-Shot Multiplex SRS for Rapid Chemical Imaging: Microplastics, FFPE Virtual Histology, and Broader QC Applications

***Eric Michele Fantuzzi*[1], Federica Padelli[2], Tiago Azevedo[3], Federico Monti[1], Gabriele Di Noia[1], Anna Muhlig[4], Orlando Guntinas Lichius[4], Rebeca Martinez Vasquez[5], Alessandra Nardini[2], Pietro Liò[3], Giulio Cerullo[2], Francesco Crisafi[1]**

[1]*Cambridge Raman Imaging Srl, Via Durando 39, 20158, Milan, Italy*
[2]*Politecnico di Milano, Dipartimento di Fisica, P.zza Leonardo da Vinci 32, 20133, Milan, Italy*
[3]*Department of Computer Science and Technology, University of Cambridge, Cambridge, UK*
[4]*Jena University Hospital, Am Klinikum 1, 07747 Jena, Germany*
[5]*CNR IFN, P.zza Leonardo da Vinci 32, 20133, Milan, Italy*

Single-shot multiplex Stimulated Raman Scattering (SRS) provides simultaneous chemical and morphological contrast with the speed required for both environmental monitoring and biomedical workflows. We describe a broadband single-shot multiplex SRS system that captures 38 spectral channels across the C–H stretching region (2800–3100 cm^{-1}) in a single acquisition within microseconds while maintaining high spatial resolution, avoiding sequential spectral scanning.

We evaluated the system for multiple application domains. For environmental analysis, we demonstrate identification and quantification of microplastic particles deposited on microscope slides and membrane filters and show in-flow detection in aqueous silica flow cells. Measurements were used to build a reference spectral library to support automated classification and counting. For biomedical microscopy, hyperspectral SRS images of FFPE sections were co-registered with conventional H&E; a convolutional neural network produced virtual H&E–equivalent images and a downstream model performed semantic segmentation to annotate tissue structures, including tumour regions. The histology workflow was tested on FFPE samples including head and neck, intestine, ocular bulbs, and breast tissue, with expert review indicating strong concordance to standard histology.

Beyond these demonstrations, the multiplex SRS acquisition strategy is applicable to other quality-control and imaging tasks (for example, pharmaceutical tablet QC and cytology), where rapid, label-free chemical contrast and throughput are advantageous.

The system demonstrated robust performance across diverse, representative sample sets. Inter-instrument consistency assessments and expansion of the reference library are underway to support broader reproducibility and deployment. Overall, single-shot multiplex SRS combined with automated analysis offers a versatile, scalable approach for rapid, reagent-free chemical imaging across environmental, biomedical, and industrial applications.

Keywords: multiplex SRS, microplastics, FFPE, virtual H&E, pharmaceutical QC, cytology

Oral Abstracts

[Abstract:0093] [SERS/TERS/Plasmonics]

Chirality Conferral Enables the Observation of Hyper-Raman Optical Activity

***John Kerr*[1], *Robin Jones*[1], *Hyunah Kwon*[2], *Ruidong Ji*[1], *Emilija Petronijevic*[4], *Liwu Zhang*[5], *Dan Pantoş*[3], *Tim Batten*[6], *Peer Fischer*[2], *Daniel Wolverson*[1], *David Andrews*[7], *Ventsislav Valev*[1]**

[1]*Department of Physics, University of Bath, Bath, BA2 7AY, UK*
[2]*Max Planck Institute for Medical Research, Jahnstr. 29, 69120 Heidelberg, Germany*
[3]*Department of Chemistry, University of Bath, Bath, BA2 7AY, UK*
[4]*SBAI Department, La Sapienza University of Rome, Rome, 00161 ROMA, Italy*
[5]*Department of Environmental Science and Engineering, Fudan University, Shanghai, 200433 China*
[6]*Renishaw plc, New Mills, Kingswood, Wotton-under-Edge GL12 8JR, UK*
[7]*School of Chemistry, University of East Anglia, Norwich Research Park, Norwich, NR4 7TJ, UK*

Chirality detection using Raman scattering, Raman optical activity (ROA), is a widely understood and respected method. However, chirality detection using hyper-Raman scattering, hyper-Raman optical activity (HROA), has remained elusive due to its requirement of frequency doubling coupled with a vibrational transition. Here we use chirality conferral between a nanohelical surface enhanced Raman scattering substrate and an achiral analyte to demonstrate first detection of HROA since its prediction in 1979.

Chirality conferral is fundamental for understanding the origin of life and is of direct importance for synthesizing new pharmaceuticals. Human-made, self-assembling nanostructures replicate the biological chirality conferral processes utilizing covalent and non-covalent bonds. However, chirality conferral from one form of matter to another via electromagnetic fields is more subtle and less explored.

We report chirality conferral between gold (Au) nanohelices and achiral molecules (crystal violet) which was designed as doubly resonant, with the nanohelices and molecules resonating at the fundamental frequency and at the second-harmonic, respectively. This enabled the experimental observation of HROA since it was first predicted 47 years ago [J. Chem. Phys. 1979, 70, 1027–1030].

Fig 1A shows an illustration of left-handed Au nanohelices coated in crystal violet being illuminated by left- and right-handed circularly polarized (LCP and RCP) light to detect any circular intensity difference from the Raman and hyper-Raman spectra of the anolyte. Doing this reveals that the achiral anolyte coated onto differently handed nanohelices produce hyper-Raman circular intensity spectra of opposite sign, see Fig 1B. By illuminating the samples with LCP and RCP for eight sample orientations and seeing no change in the sign of the Raman spectra, we demonstrate the effect originates from intrinsic chirality. Our results demonstrate that field-driven chirality conferral mechanisms are opening entire fields of ROA research, as exemplified by the discovery of this physical phenomenon.

Keywords: Hyper-Raman, Chirality, ROA, SERS

Figure 1

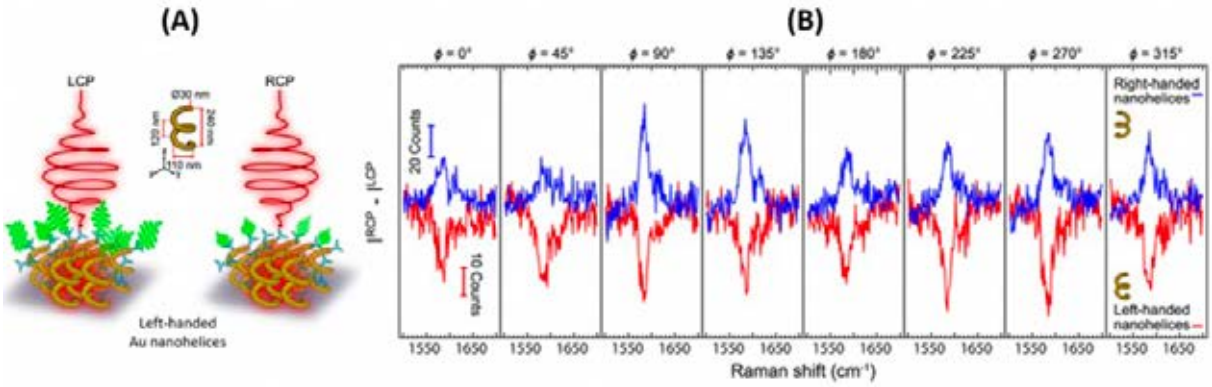


Fig. 1. (A) Diagram of the reported HROA effect: illumination with left- and right-handed circularly polarized (LCP and RCP) light results in different intensities of hyper-Raman scattering. (B) Surface enhanced hyper-Raman scattering – circular intensity difference spectra are plotted for eight sample orientations. The circular intensity difference spectra are consistently negative for CV on left-handed nanohelices (in red) and positive for CV on right-handed nanohelices (in blue). [Nat. Photon. 2024, 18, 982–989]

[Abstract:0094] [Materials]

Polarised Raman and Second Harmonic Generation Microscopy for Probing Symmetry, Strain, and Layer Interactions in Two Dimensional Materials

Iona Elizabeth Hill

Edinburgh Instruments, Livingston, UK

Understanding the structural and electronic properties of two dimensional (2D) materials requires characterisation techniques that are both non destructive and highly sensitive to crystal symmetry, interlayer coupling, and local variations in strain or defects. In this work, we demonstrate how the combined use of polarised Raman spectroscopy and second harmonic generation (SHG) microscopy enables powerful multimodal analysis of 2D materials.

Polarised Raman spectroscopy provides orientation dependent phonon responses that allow determination of crystal axes, identification of polytype variations, and mapping of strain or doping heterogeneity with sub micron spatial resolution. Complementary SHG imaging offers symmetry specific contrast that is highly sensitive to layer number, grain boundaries, and rotational domains, enabling rapid visualisation of crystal quality across large sample areas.

By correlating SHG and Raman signatures, we obtain insights that would be inaccessible to either technique alone. SHG maps guide the interpretation of polarisation resolved Raman measurements, while Raman peak shifts and intensity variations reveal mechanical or electronic changes that are not SHG active. Together, these modalities provide a coherent framework for quantitatively assessing growth quality, domain orientation, and local structural variations in emerging 2D heterostructures. This multimodal approach supports the development of reproducible, scalable characterisation workflows essential for integrating 2D materials into next generation optoelectronic, quantum, and photonic devices.

Keywords: Raman Spectroscopy, Second Harmonic Generation, Two-Dimensional Materials, Polarised Raman

Oral Abstracts

[Abstract:0096] [Theory/Computation]

Vibrational Spectroscopy Under External Electric Fields: Probing Molecular Structure and Interactions

***Matteo Tommasini*[1], *Franz Saija*[2], *Sebastiano Trusso*[2], *Giuseppe Cassone*[2]**

[1]*Dipartimento di Chimica, Materiali e Ingegneria Chimica "G. Natta", Politecnico di Milano, Milano, Italy; CNR-IPCF, Istituto per i Processi Chimico-Fisici, Messina, Italy*
[2]*CNR-IPCF, Istituto per i Processi Chimico-Fisici, Messina, Italy*

The interaction between molecules and intense, oriented external electric fields provides a useful framework for understanding how electric perturbations affect structure, bonding, and spectroscopy in a wide range of chemical systems. By combining high-level quantum-chemical methods and vibrational analysis, one can explain how external fields affect both intermolecular interactions and the intrinsic properties of conjugated chromophores. Therefore, Raman and infrared (IR) spectroscopy are sensitive tools for detecting field-induced polarization, symmetry breaking, and bond strengthening [1-4]. In noncovalent systems like hydrogen- and halogen-bonded dimers [1-3], electric fields aligned with the donor–acceptor axis typically strengthen intermolecular interactions. This increase is reflected by systematic vibrational Stark shifts, especially for stretching modes related to the bond donor. These findings demonstrate that vibrational frequency shifts can accurately indicate changes in noncovalent bond strengths due to external perturbations.

Applying the same approach to π-conjugated molecules emphasizes the importance of symmetry and permanent dipole moments. Indigo [4] is a classic example of a centrosymmetric system in which Raman and IR activities are mutually exclusive under zero-field conditions. When an external electric field is applied, inversion symmetry is broken, a finite dipole moment is generated, and Raman modes also become IR-active (and vice versa). In this context, the vibrational Stark effect appears not only as frequency shifts but also as a redefinition of selection rules, where the changes in intensity offer direct insights into local electric fields.

Violacein provides a complementary example to Indigo. As a non-centrosymmetric, permanently polar chromophore, Violacein shows a strongly nonlinear dipole and polarizability response under oriented fields. The vibrational Stark effect is particularly significant for specific C=C stretching modes. Charge redistribution caused by the field, along with conformational changes, greatly influences both Raman and IR intensities.

Overall, these results present a clear picture: electric fields influence bond strength and electron distribution, vibrational Stark shifts reflect energetic changes, and molecular symmetry determines how these effects manifest spectroscopically. Raman and IR spectroscopy can thus serve as powerful, field-sensitive tools for investigating electric environments in complex chemical and biological systems.

References:

[1] https://doi.org/10.1021/acs.jpca.5c08038

[2] https://doi.org/10.1021/acs.jpca.4c01553

[3] https://doi.org/10.1021/acs.jpca.5c01095

[4] https://doi.org/10.1021/acs.jpca.0c09791

Keywords: Violacein, Density Functional Theory, Oriented Electric Fields, Vibrational Stark Shift

[Abstract:0101] [SERS/TERS/Plasmonics]

Temporal Fluctuations in SERS Signals Revealed by DBSCAN-Based Cluster Analysis

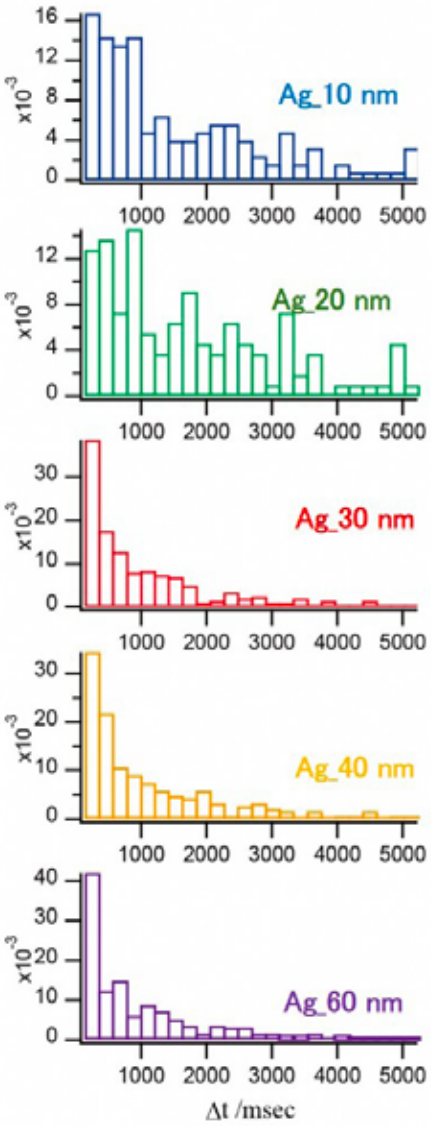
***Yuika Saito*, Yuki Takeuchi, Kota Uchiyama, Ayane Ganaha, Takahiro Kondo**

Department of Chemistry, Gakushuin University

We investigated the temporal fluctuations of surface-enhanced Raman scattering (SERS) spectra from a small number of molecules with a temporal resolution of 25 ms using a conventional EMCCD-based setup. To improve the signal-to-noise (S/N) ratio of the time-resolved spectra, we applied density-based spatial clustering of applications with noise (DBSCAN). This approach enabled clearer discrimination between SERS ON and OFF states, which were otherwise difficult to classify due to the low S/N ratio. The analyte was an aqueous solution of crystal violet, and silver nanoparticles (AgNPs) with diameters ranging from 10 to 60 nm were used as SERS substrates. A ×60, NA 0.7 objective lens was employed, and approximately 15 crystal violet molecules were present within the laser focal volume. Spectra were acquired with a 10 ms accumulation time under continuous-wave 532 nm laser excitation. As shown in Figure 1, we quantitatively analyzed ON/OFF dynamics using histograms of ON-time intervals (Δt). The histogram characteristics varied with particle size, nanoparticle density, and specific Raman vibrational modes. Notably, the fluctuation behavior differed between in-plane and out-of-plane vibrational modes. The temporal behavior of the SERS signals exhibited a strong dependence on nanoparticle size and was well described by a two-dimensional random-walk model. In this model, AgNPs diffuse into and out of the laser focal volume, and SERS signals are detected only when a nanoparticle enters the focus. This indicates that the primary source of fluctuation is the Brownian motion of the AgNPs. In addition to intensity fluctuations, we analyzed frequency shifts in several Raman bands using histograms of Δwavenumber/Δt. The quadrupole mode influenced the frequency fluctuations in larger AgNPs. The 1181 cm^{-1} mode, which consists of two closely overlapping vibrations with distinct symmetries, exhibited numerous high-frequency components, in contrast to the single-component 914 cm^{-1} mode. Overall, our findings demonstrate the utility of combining SERS with DBSCAN for probing nanoscale dynamics and highlight its potential for advancing analytical and biological applications of nanoparticle-based SERS.

Keywords: SERS, DBSCAN Cluster Analysis, Temporal Fluctuation

Figure1



Histograms of ON-time intervals (Δt) for 914 cm^{-1} mode

Oral Abstracts

[Abstract:0102] [SERS/TERS/Plasmonics]

Force-Induced Isomerization of Azobenzene Monitored by Tip-Enhanced Raman Spectroscopy

***Balaji Sanap*[1], *Abhinav Sharma*[1], *Takuo Tanaka*[2], *Taka Aki Yano*[1]**

[1]*Tokushima University, Minami-Jyosanjima, Tokushima, Japan*
[2]*RIKEN, 2-1 Hirosawa, Wako, Saitama, Japan*

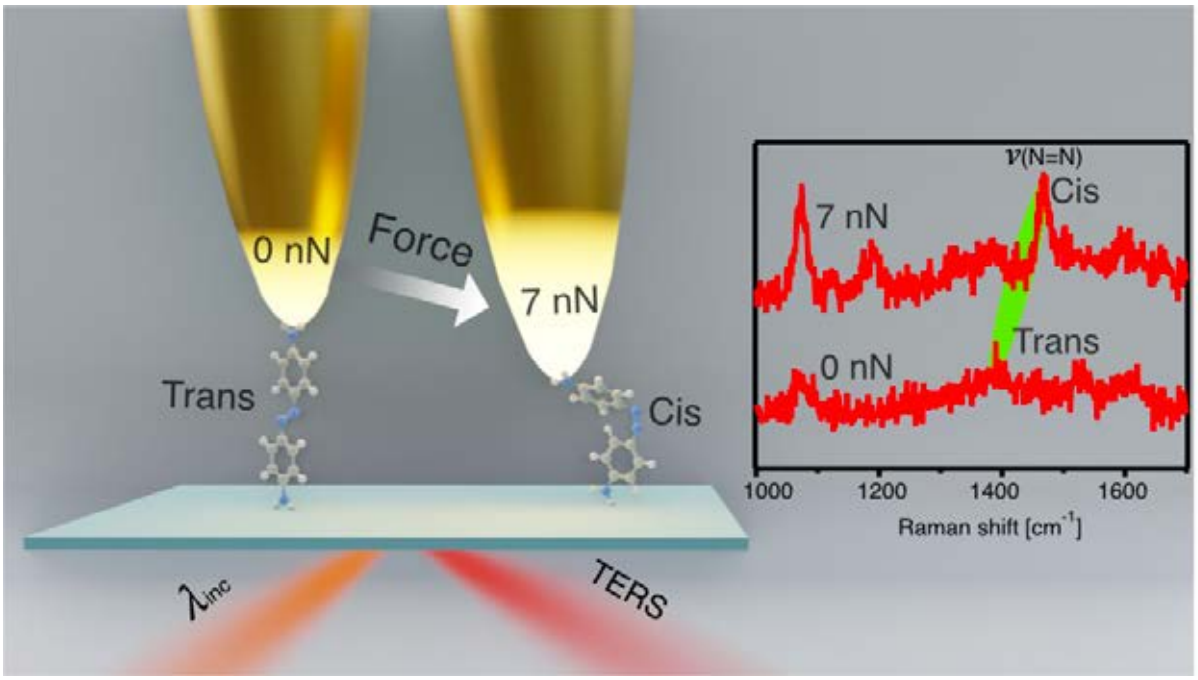
Tip-enhanced Raman spectroscopy (TERS) has emerged as a powerful nanoscale vibrational tool capable of probing molecular fingerprints with single molecular sensitivity through highly confined field at the tip-substrate junction. Beyond spectroscopic detection, the localized tip-molecule interaction enables investigation of molecular transformations under applied mechanical stimuli, providing a direct insight into molecular transformations at nanoscale through vibrational signatures. To explore this capability, molecular system capable of undergoing structural switching are particularly attractive for studying such mechanically driven process. Among such systems, azobenzene is well-studied photo-switchable molecule which undergoes reversible trans-cis isomerization through the rearrangement around N=N bond. Although the switching behaviors extensively studied under photoexcitation, direct monitoring of isomerization driven purely mechanically confirmed through vibrational fingerprints remains largely unexplored.

In this study, we demonstrate the mechanically induced isomerization of azobenzene probed by application of force through metallic tip and observed in-situ with changes in vibrational fingerprints. As schematically illustrated in figure. 1, Diamino-azobenzene (DAAB) molecule is sandwiched between the metallic flat substrate and tip, forming a plasmonic nanogap. The inset of the TERS spectra clearly distinguishes the trans- and cis- confirmations through the shift in $\mathcal{V}$(N=N) vibrational mode upon force application, confirming the structural transformation of azobenzene. The tip-applied mechanical stimuli supply sufficient energy to drive trans-cis transformation.

These findings highlight the potential of the TERS to induce isomerization of azobenzene and ability to observe through the spectral changes upon isomerization. This study provides new inisghts into understanding of mechanochemical transformation of molecules at nanoscale. Such insights open new opportunities for studying molecular mechanochemistry and controlling chemical process at single molecular level.

Keywords: Tip-enhanced Raman spectroscopy, mechanochemistry, isomerization

Figure1



TERS nanojunction between a metallic tip and a flat metallic substrtae with the DAAB molecule in between. Inset: corresponding TERS spectra from nanojunction

[Abstract:0103] [Novel Approaches]

Meta-Raman Optical Activity

Ventsislav K. Valev

Department of Physics, University of Bath, Bath, UK

Raman optical activity (ROA) provides vibrationally resolved chiral contrast, yet conventional molecular ROA is exceptionally weak and highly susceptible to polarimetric artifacts. Chiral plasmonic nanostructures have therefore been explored both as surface-enhanced Raman scattering (SERS) substrates and as platforms for chirality conferral. In earlier work on dense arrays of ~100 nm gold nanohelices functionalized with nominally achiral crystal violet, we observed circular-intensity differences in SERS and subsequently demonstrated hyper-Raman optical activity under doubly resonant conditions.[1,2] By establishing rotation invariance and excluding extrinsic chirality, those studies showed that electromagnetic near fields of chiral nanohelices can confer chirality to an achiral molecular response.

Here we place these findings in a unified and more stringent polarimetric framework and demonstrate metasurface-mediated ROA (meta-ROA): ROA-like, polarization-resolved Raman observables that arise from near-field–mediated polarization transfer in a hybrid molecule–metasurface system, rather than from molecular chirality. Using enantiomeric arrays of gold and silver nanohelices functionalized with crystal violet and rhodamine 6G, we implement a polarization-resolved Raman microscope achieving high-purity circular polarization at the sample plane, verified by in situ polarimetry, with dual circular selection in both excitation and detection.

By measuring all four circular in→out scattering channels and constructing the complete circular polarization transfer matrix, we access Barron-style ROA at Stokes/anti-Stokes frequencies and Nafie-style observables (DCP_1 and DCP_2). All observables exhibit mutually consistent handedness and reverse sign upon switching nanohelix handedness, providing internal validation and rigorous artifact control. The differential signals reach ~10%, orders of magnitude larger than typical molecular ROA.

References:

[1] R. R. Jones, J. F. Kerr, H. Kwon, S. R. Clowes, R. Ji, E. Petronijevic, L. Zhang, G. Dan Pantoș, B. Smith, T. Batten, P. Fischer, D. Wolverson, D. L. Andrews, V. K. Valev, Chirality conferral enables the observation of hyper-Raman optical activity. Nat. Photonics 18, 982–989 (2024).

[2] R. R. Jones, C. Miksch, H. Kwon, C. Pothoven, K. R. Rusimova, M. Kamp, K. Gong, L. Zhang, T. Batten, B. Smith, A. V. Silhanek, P. Fischer, D. Wolverson, V. K. Valev, Dense arrays of nanohelices: Raman scattering from achiral molecules reveals the near-field enhancements at chiral metasurfaces. Adv. Mater. 35, 2209282 (2023).

Keywords: Raman optical activity, plasmonics, SERS, SEROA, metasurface

Oral Abstracts

[Abstract:0104] [SERS/TERS/Plasmonics]

Natural Hyperbolic $MoOCl_2$ for Anisotropic Raman and SERS-Like Enhancement

***Anton Minnekhanov*[1], *Georgy Ermolaev*[1], *Gleb Tselikov*[1], *Aleksey Arsenin*[1], *Valentyn Volkov*[1], *Kostya Novoselov*[2]**

[1]*Emerging Technologies Research Center, XPANCEO, Dubai, United Arab Emirates*
[2]*National Graphene Institute (NGI), University of Manchester, Manchester, U.K.*

Hyperbolic electromagnetic response can be engineered in anisotropic metamaterials, while naturally occurring hyperbolic crystals are comparatively rare and often operate in the mid-infrared.[1,2] Here we present $MoOCl_2$, a layered van der Waals material[3] with extreme in-plane anisotropy (metallic along the a-axis and dielectric along the b-axis), as a natural platform that brings hyperbolic physics into the visible/near-infrared window relevant for Raman spectroscopy and SERS.

Angle-resolved polarized Raman spectroscopy of $MoOCl_2$ reveals a strongly direction-dependent coupling between phonons and an electronic continuum. For excitation polarized along the metallic axis, several phonons acquire pronounced Fano asymmetry, consistent with interference between discrete phonons and an electronic Raman scattering continuum. Rotating the polarization toward the dielectric axis suppresses this asymmetry and redistributes the Raman intensity between modes, providing a clear spectroscopic signature of anisotropic electron-phonon coupling and a practical way to identify crystallographic axes.

We then exploit the same anisotropic optical response for "Hyperbolic-Enhanced Raman" (HypER) sensing on exfoliated $MoOCl_2$ flakes, without lithography or noble-metal nanoparticles. Molecular analytes deposited on $MoOCl_2$ exhibit large, polarization-tunable Raman enhancement with an intrinsic on/off contrast controlled by aligning the incident polarization with the metallic axis. In addition to benchmark dyes, we observe analogous SERS-like performance for pharmacologically relevant molecules such as doxorubicin, supporting broader applicability for chemical and bio-analytical sensing.

Finally, we show that $MoOCl_2$ acts as a Raman booster substrate for other low-dimensional materials. When MoS_2 and WS_2 are transferred onto $MoOCl_2$, their characteristic Raman modes are enhanced by tens of times compared with standard dielectric substrates, and the enhancement inherits the in-plane anisotropy of the hyperbolic host. This hybrid approach enables boosted Raman readout of 2D heterostructures while adding polarization selectivity as an extra contrast channel.

These results connect hyperbolic van der Waals materials and SERS-style enhancement, and suggest $MoOCl_2$ as a simple, polarization-programmable substrate for molecular sensing and Raman studies of 2D materials.

References:

[1] Poddubny A. et al., 7, 948 (2013)

[2] Basov D. et al., Science, 354, aag1992 (2016)

[3] Venturi G. et al., Nat. Commun., 15, 9727 (2024)

Keywords: hyperbolic materials, SERS, anisotropy, van der Waals materials, 2D materials, MoOCl2

Oral Abstracts

[Abstract:0107] [Biology/Biomedicine]

Dielectrophoresis Enhancement of Raman Spectroscopy in Liquid for Biological Characterizations: Viruses, Bacteria and Eco-Coronas on Nanoplastics

***Alessio Sacco*[1], *Camilla Sacco Botto*[2], *Anna Placci*[3], *Marta Fadda*[1], *Slavica Matic*[2], *Simona Ortelli*[4], *Valentina Marassi*[3], *Raquel Portela*[5], *Emanuela Noris*[2], *Andrea Mario Giovannozzi*[1], *Chiara Portesi*[1], *Andrea Mario Rossi*[1]**

[1]*Quantum Metrology and Nanotechnology, Istituto Nazionale di Ricerca Metrologica (INRiM), Torino, Italy*
[2]*Istituto per la Protezione Sostenibile delle Piante, Consiglio Nazionale delle Ricerche (IPSP-CNR), Torino, Italy*
[3]*Dipartimento di Chimica "Giacomo Ciamician", Università di Bologna, Bologna, Italy*
[4]*Istituto di Scienza, Tecnologia e Sostenibilità per lo Sviluppo dei Materiali Ceramici, Consiglio Nazionale delle Ricerche (ISSMC-CNR), Faenza, Italy*
[5]*Instituto de Catálisis y Petroleoquímica, Consejo Superior de Investigaciones Científicas (ICP-CSIC), Madrid, Spain*

Raman spectroscopy boasts to be a label-free, non-destructive analytical technique that necessitates little sample preparation, ideal for biological applications such as the measurement of living tissues, bacteria, viruses, and biomolecules. However, its growing uses, including declinations such as surface-enhanced Raman, often face limitations like surface selectivity or the need for sample drying.

To overcome Raman's sensitivity limitations, dielectrophoresis (DEP) represents a compelling strategy. DEP is a physical phenomenon in which non-uniform electric fields result in net forces on polarizable particles, such as cells and macromolecules. Leveraging DEP in liquid allows the sample to agglomerate in the confocal volume of the Raman microscope, locally maximizing concentration in a reversible, tunable process, allowing measurements in liquid in seconds, with unprecedented sensitivity and with the possibility to selectively separate samples from contaminants. In this work, some novel applications of DEP-aided Raman are presented.

DEP-Raman was employed to identify different viruses in suspension, and to rapidly detect dynamic changes of the tobacco mosaic virus (TMV) protein envelop by thermic treatments; the transition and loss of infectivity were confirmed by transmission electron microscopy and plant inoculation.

A study on DEP-Raman for the identification of bacteria at sub-species level is also demonstrated. Machine learning techniques were applied on Raman spectra acquired on plant bacteria concentrated by DEP in culture medium, allowing identification of pathovars with accuracies, precisions, recalls, and F1 scores of 94–100%.

Finally, DEP-Raman was applied to study PET nanoplastics after interacting with pollen. It selectively accumulated and measured pollen, separating it from isolated nano-PET in protein-rich suspension, demonstrating that pollen can form complex structures with nanoplastics and carry them. The resulting eco-corona formation detection was corroborated by techniques such as field-emission scanning electron microscopy, field-flow fractionation, and pyrolysis-gas chromatography-mass spectrometry.

Classification of pathogens is of utmost importance, but current diagnosis is mainly based on time-consuming and expensive serological and molecular methods. Nanoplastics analysis is very unexplored due to lack of impactful analytical techniques, and eco-corona formation on nanoplastics impacts their airborne transportation and bioaccumulation. By providing a rapid, flexible analytical technique, DEP-Raman can unlock new analytical possibilities in the biological field.

Keywords: Biological samples, bacteria, viruses, ecocorona, nanoplastics, dielectrophoresis

[Abstract:0112] [Novel Approaches]

Online Coupling of Size Exclusion Chromatography to Capillary Enhanced Raman Spectroscopy for Biopharmaceutical and Biological Applications

***Jana Thissen*[1], *Martin D. Klassen*[1], *Michael C. Hacker*[2], *Joerg Breitkreutz*[2], *Thorsten Teutenberg*[1], *Björn Fischer*[2]**

[1]*Institut für Umwelt & Energie, Technik & Analytik e.V. (IUTA), Bliersheimer Straße 58-60, 47229 Duisburg, Germany*
[2]*Institute of Pharmaceutics and Biopharmaceutics, Faculty of Mathematics and Natural Sciences, Heinrich Heine University, Universitätsstraße 1, 40225 Düsseldorf, Germany*

The coupling of liquid chromatography (LC) with spectroscopic techniques such as UV/Vis spectroscopy has been well established since the 1980s. In contrast, the online combination of LC with Raman spectroscopy (RS) has been explored only to a limited extent. RS provides structural information on proteins, including conformational features, enabling non-destructive and label-free analysis under native conditions. To date, most studies have focused on pure compounds or defined mixtures analyzed by RS following chromatographic separation, rather than on analytes within complex biological matrices.

The aim of this work was therefore to investigate the potential and limitations of online LC–RS coupling for the analysis of proteins and their prosthetic groups in biopharmaceutical and biological samples, addressing relevant bioanalytical challenges. Size exclusion chromatography (SEC) was selected as the separation technique due to its importance in biopharmaceutical characterization. The instrumental setup of the coupled system is described in detail, particularly the capillary based flow cell that enables capillary-enhanced Raman spectroscopy (CERS).

The developed SEC–CERS system was successfully applied to the structural elucidation and identification of various proteins in samples such as biopharmaceutical formulations and blood serum. The method enabled simultaneous assessment of therapeutic protein conformation and quantification of functional excipients, potentially supporting the comprehensive characterization required by regulatory authorities. In hemolyzed serum, the biomarkers serum albumin, immunoglobulin G, and hemoglobin were successfully identified. Automated data processing combined with principal component analysis allowed differentiation of three biotherapeutic IgG1 antibodies, both, as pure active substances and in combination with their respective excipients, highlighting the method's potential for pharmaceutical quality control through discrimination and similarity assessment of protein samples.

In summary, this work presents several practical applications of SEC–CERS for protein analysis and demonstrates a substantial contribution to advancing Raman spectroscopic detection in liquid chromatography.

Keywords: Online coupling, Size Exclusion Chromatography, Liquid Core Waveguide, Biopharmaceutical analysis, Peptides and Proteins

Oral Abstracts

[Abstract:0113] [Novel Approaches]

Development of Macro- and Microscale Line-Scan Raman Systems for Environmental Monitoring

Hyung Min Kim

Department of Chemistry, Kookmin University, Seoul, Korea

Raman spectroscopy offers unparalleled potential for the chemical identification of microplastics (MPs); however, the technique is fundamentally constrained by spectral acquisition speed and the difficulty of signal collection from morphologically complex and sub-diffraction-limited samples. This study presents two advanced Raman spectroscopic architectures designed to overcome the physical challenges of signal acquisition in heterogeneous environmental matrices.

We first demonstrate a line-scan Raman imaging platform optimized for capturing spectral and spatial information on 47 mm filter surfaces. [J. Hazard. Mater. 2025, 499, 1, 140101] By engineering the laser excitation profile, we effectively mitigate the signal variance caused by uneven topography, achieving high-fidelity Raman mappings of 10-μm-scale particles. The integration of high-speed mosaic scanning allows for efficient photon collection over large surface areas. Furthermore, we present a flow-based Raman plastometry platform employing optical line tweezers. [ACS Sensors 2026, online publication] This approach utilizes radiation pressure to provide precise optical immobilization of particles, effectively overcoming the diffusive dynamics of sub-micron MPs (500 nm). By confining particles within the focal volume via optical traps, we demonstrate the ability to acquire high-quality Raman spectra with improved signal-to-noise ratios, even in dynamic liquid environments. These advancements in Raman instrumentation—ranging from beam-profile engineering for surface scanning to optical potential manipulation for microfluidic sensing—provide new methodologies for pushing the limits of Raman-based microplastic analysis.

Keywords: Line-scan, Raman, Microplastics, in situ, in aquo

[Abstract:0114] [Coherent Raman Imaging]

Highly Sensitive and Fast Hyperspectral SRS Image Acquisition as Well as TPE Microscopy with Shot Noise Limited OPO-Based Light Source

***Ingo Rimke*[1], *Rene Siegmund*[2], *Maryam Sanaee*[3], *Jerker Widengren*[3], *Alexander Egner*[2], *Gero Stibenz*[1]**

[1]*APE GmbH, Berlin, Germany*
[2]*Department of Optical Nanoscopy, Institute for Nanophotonics Göttingen, Germany*
[3]*Royal Inst. Technology (KTH), Dept Applied Physics, Stockholm, Sweden*

We report on recent developments in commercial picosecond light sources designed for ultra-sensitive Stimulated Raman Scattering (SRS) imaging, targeting both the fingerprint spectral region and Raman labels. By halving the repetition rate to 40 MHz and implementing additional optimizations, we achieved a tenfold improvement in image acquisition speed over the previous system generation. Together with shot-noise-limited performance it enables SRS imaging of compounds at biologically relevant concentrations.

The light source delivers several hundred milliwatts of output power, with a spectral bandwidth of approximately 10 cm^{-1} and a pulse duration of 2 ps for both Pump and Stokes beams, covering a broad spectral range of 210–5450 cm^{-1}. This encompasses all relevant vibrational bands at sufficient spectral resolution. Rapid wavelength tuning across the entire range in approximately two seconds facilitates straightforward multispectral SRS imaging. The system operates in a fully automated, hands-free manner, with built-in spatial and temporal co-alignment of Pump and Stokes beams to guarantee optimal overlap at the sample.

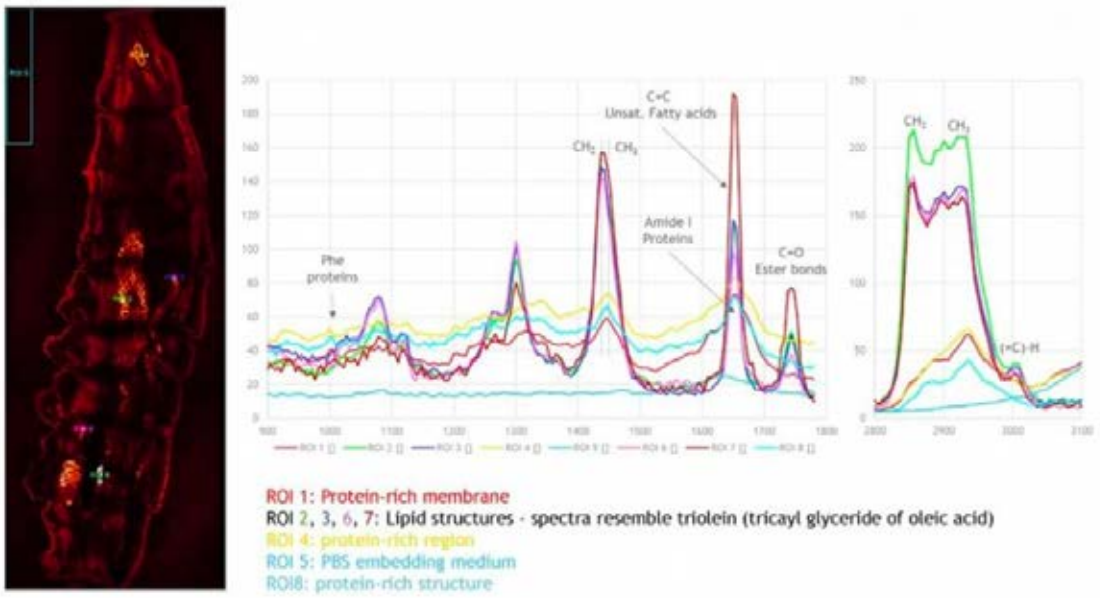
We present benchmark measurements demonstrating the improvements in sensitivity and acquisition speed, along with multispectral SRS imaging of biological samples in the fingerprint region and Raman label imaging.

To meet the distinct demands of Coherent Raman microscopy — which requires high chemical specificity — and two-photon excitation (TPE) microscopy — which benefits from shorter pulses for efficient excitation — we implemented a dedicated OPO configuration producing a broader bandwidth of 30 cm^{-1} instead of 10 cm^{-1}. These pulses are compressed to approximately 400–500 fs, making them well-suited for TPE microscopy. Seamless switching between the two operational modes is demonstrated.

Keywords: SRS microscopy, OPO-based light source, CRS imaging

Oral Abstracts

Leica STELLARIS CRS microscope with the picoEmerald FT: Fast spectroscopic SRS imaging of hatched drosophila larvae



[Abstract:0115] [SERS/TERS/Plasmonics]

Hemispherical Gold Nanoshell Arrays on Silicon Nanospheres for Single-Digit Nanogap SERS Substrates

***Taeyeong Kim*, Jungchul Lee**

Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology, Daejeon, South Korea

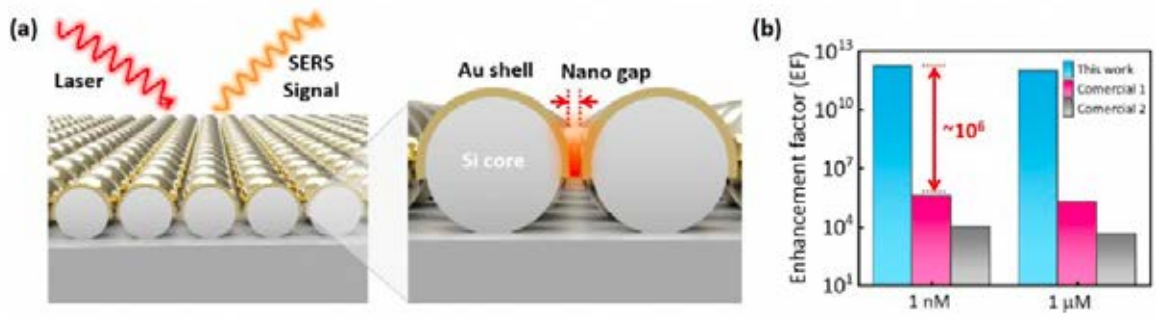
Surface-enhanced Raman scattering (SERS) enables highly sensitive molecular detection by amplifying Raman signals at plasmonic hotspots. For practical sensing and quantitative analysis, SERS substrates require highly uniform nanogaps over large areas. Even small gap variations can produce large spot-to-spot fluctuations in electromagnetic enhancement and Raman intensity. Achieving this level of uniformity at wafer scale, while maintaining scalable throughput, remains a key challenge. Here we present a two-step strategy that combines localized laser processing of silicon nanopillar arrays with thin-film deposition to form hemispherical gold nanoshell arrays featuring single-digit nanogaps at a sub-micrometer pitch (Fig. 1a).

Silicon nanopillar arrays were fabricated by deep-UV stepper lithography and dry etching, yielding a diameter of 100 nm, a spacing of 100 nm, and an aspect ratio of 3. Laser processing was then done in vacuum, where an out-of-plane thermal gradient drives directional surface atom transport and reshapes cylindrical pillars into silicon nanospheres. By tuning the processing conditions, the inter-feature spacing is controllably reduced during spheroidization, producing dense nanosphere arrays with characteristic structural colors that track the size evolution. Subsequently, electron-beam evaporation of a thin gold film forms hemispherical nanoshells on the nanospheres, further narrowing inter-shell separations down to a minimum 1 nm scale across the array.

SERS performance was evaluated using rhodamine 6G (R6G) at two concentrations (1 nM and 1 μM), and the enhancement factor (EF) was quantitatively determined. The 1 nm-scale inter-shell gaps yield EF values exceeding 10^{12}, corresponding to an approximately 10^6-fold improvement over two high-performance commercial SERS substrates measured under identical conditions (Fig. 1b). Importantly, wafer-scale mapping confirms that this high performance is preserved across the entire wafer area, with Raman signal non-uniformity remaining within 5%, demonstrating highly uniform, wafer-wide hotspot reproducibility.

Keywords: Surface-enhanced Raman scattering (SERS), Nanogap, Wafer-scale, Laser annealing, Shape evolution

Figure 1



(a) Hemispherical Au nanoshell arrays on Si nanospheres forming 1 nm inter-shell nanogaps for SERS hotspots. (b) R6G SERS enhancement factors at 1 nM and 1 μM, showing EF > 10^{12} and ~10^6 higher performance than commercial substrates.

[Abstract:0118] [Biology/Biomedicine]

Raman Spectral Cytopathology: A Minimally Invasive Approach for Early Detection of Pre-Cancerous Lesions

Fiona Lyng

Radiation and Environmental Science Centre, Physical to Life Sciences Research Hub, FOCAS Building, Technological University Dublin, Dublin, IRELAND; School of Physics, Clinical and Optometric Sciences, Technological University Dublin, Dublin, IRELAND

Early detection of pre-cancerous lesions provides a critical opportunity to intervene and prevent cancer before it even develops. This forms the basis for screening programmes for several cancers in most developed countries. Cervical screening, for example, employs HPV testing and cytopathology of exfoliated cells collected using a cytobrush. However, the current gold-standard approaches, cytopathology and histopathology, have notable limitations, including subjectivity, cost and long turnaround times. As well as missed diagnosis, overdiagnosis and overtreatment can also occur, as it can be challenging to identify pre-cancerous lesions likely to progress to cancer. There is a clear unmet need for complementary techniques that can support clinicians in the early detection of pre-cancerous lesions or potentially malignant lesions where malignant transformation has not yet occurred. Minimally invasive approaches, such as brush biopsy of exfoliated cells, can reduce the need for multiple invasive tissue biopsies in patients with pre-cancerous lesions. Raman spectroscopy offers rapid, label free and non destructive biochemical analysis of cells and tissues. While many Raman studies to date have focused on spectral histopathology, less attention has been given to spectral cytopathology. This talk will present examples of our recent work on Raman spectral cytopathology, using exfoliated cell samples for the detection of cervical and oral pre-cancerous lesions.

Keywords: Raman spectroscopy, cytopathology, oral cancer, cervical cancer, pre-cancerous lesions, exfoliated cells

[Abstract:0120] [SERS/TERS/Plasmonics]

Modulating SERS and Enhanced Fluorescence of Copper Complexes Through Silica Shell Thickness in Ag@SiO_2 Nanoparticles

***Ana Luiza Correa Januário*, Romulo Augusto Ando**

Laboratório de Espectroscopia Molecular, Instituto de Química, Universidade de São Paulo, São Paulo, Brasil

Luminescent Cu(I) complexes have attracted increasing attention due to their potential application in light-emitting devices. These complexes exhibit metal-to-ligand charge transfer (MLCT) transitions and, upon excitation, the d10 configuration undergoes a formal oxidation of copper to Cu(II), leading to excited-state geometric distortions that favor non-radiative decay pathways and reduce emission efficiency, one of the main limitations for practical applications.[1] An emerging yet underexplored strategy to mitigate this limitation in copper-based systems involves the use of metallic nanoparticles to enhance luminescence. These nanostructures support localized surface plasmon resonance (LSPR), generating intensified local electromagnetic fields capable of amplifying absorption, emission and scattering processes in nearby emmiters.[2] Herein, we systematically modulate the distance between silver nanoparticles and Cu(I) complexes to investigate how plasmonic coupling alters their photophysical properties, enabling surface-enhanced Raman scattering (SERS), surface-enhanced fluorescence with shell-isolated nanoparticles (SHINEF) or their simultaneous occurrence. Distance control was achieved by coating silver nanoparticles with silica shells (Ag@SiO_2) of varying thickness. We focused on complexes of the type [Cu(P^P)(N^N)]+, where P^P = xantphos (4,5-bis(diphenylphosphano)-9,9-dimethylxanthene) and N^N = substituted phenanthrolines. These systems exhibit MLCT absorption between 400-500 nm and emission above 500 nm (Figure 1). For [Cu(xantphos)(1,10-phenanthroline)]PF_6 in silver colloid (10^{-4} mol L^{-1}), excitation at 633 nm resulted in fluorescence quenching accompanied by pronounced SERS signal (Figure 2). In contrast, 532 nm excitation, near the MLCT absorption, resulted in selective enhancement of phenanthroline vibrational modes, consistent with a resonance SERRS mechanism (Figure 2). Using Ag@SiO_2 nanoparticles with a 10 nm silica shell under 633 nm excitation (Figure 3), solvent (acetonitrile) bands became evident, although the most intense complex modes remained observable. Under 532 nm excitation, simultaneous enhancement of SERS and SHINEF was detected. These results suggest that tuning the SiO_2 shell thickness enables optimization of the plasmon-emitter distance, potentially identifying an ideal separation that maximizes fluorescence while preserving SERS enhancement. We therefore aim to systematically elucidate structure-distance-property relationships across a series of Cu(I) complexes.

References:

[1] CrystEngComm, 2022, 24, 7739–7750

[2] Chem. Soc. Rev., 2017, 46, 3962-3979

Keywords: Copper(I) complexes, silver nanoparticles, silica, surface-enhanced fluorescence, surface-enhanced raman scattering

Figure 1

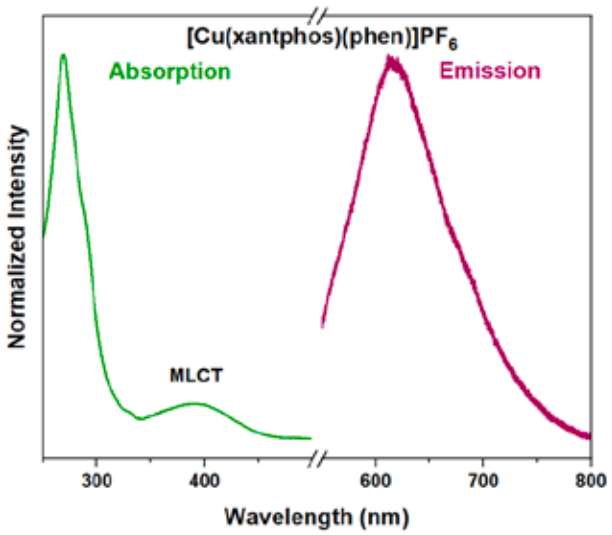


Figure 1. Normalized absorption spectrum (green) of [Cu(xantphos)(phen)]PF_6 solution (10^{-5} mol L^{-1}) and emission spectrum (red) of the solid-state complex excited at 532 nm.

Figure 2

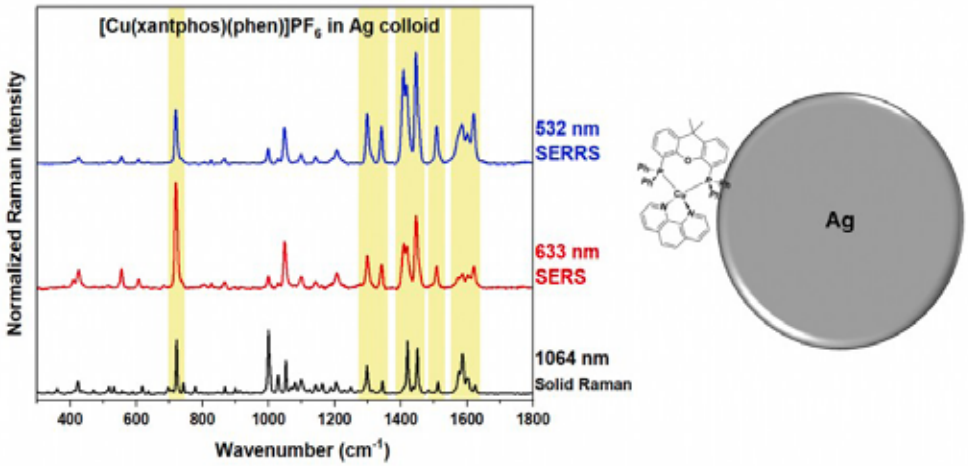


Figure 2. SERS (λ_{exc} = 633 nm) and SERRS (λ_{exc} = 532 nm) spectra of [Cu(xanthos)(phen)]PF_6 in silver colloidal solution, compared with the solid-state normal Raman spectrum (λ_{exc} = 1064 nm) (left). Schematic illustration of silver nanoparticle-complex interaction (right).

Figure 3

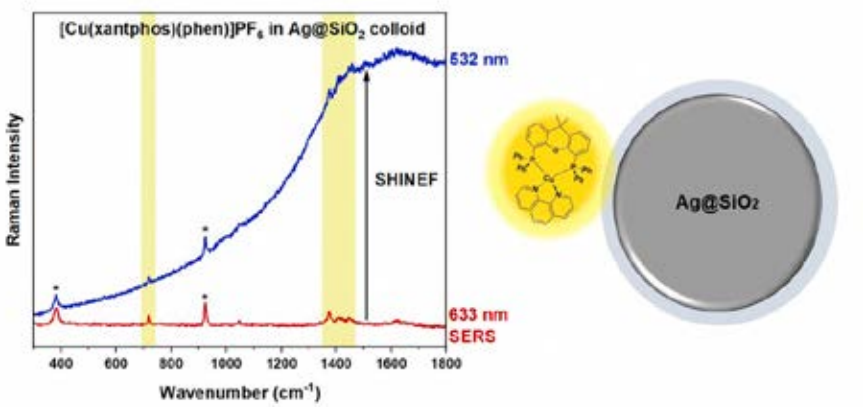


Figure 3. SERS (λ_{exc} = 633 nm) and SHINEF (λ_{exc} = 532 nm) spectra of [Cu(xanthos)(phen)]PF_6 in $Ag@SiO_2$ colloidal solution. The bands marked with an asterisk are from the solvent (acetonitrile) (left). Schematic illustration of shell-isolated silver nanoparticle-complex interaction (right).

[Abstract:0121] [Materials]

High-Field Magneto-Raman Spectroscopy of Quantum Magnets

Dmitry Smirnov

National High Magnetic Field Laboratory, Tallahassee, USA

Quantum magnets on triangular and honeycomb lattices host a rich variety of unconventional magnetic ground states and low-energy excitations arising from competing interactions and strong quantum fluctuations, making them an ideal platform for spectroscopic studies. Under extreme conditions of high magnetic fields and low temperatures, quantum phase transitions occur between distinct phases of quantum matter; simultaneously, novel low-energy magnetic excitations evolve significantly across field-driven phase boundaries. This richness motivates the development of advanced spectroscopy techniques that integrate (sub)THz-range spectral coverage with high magnetic fields, cryogenic temperatures, and polarization control. At National High Magnetic Field Laboratory (NHMFL, Tallahassee, FL), we developed a user-friendly magneto-Raman spectroscopy facility that enables polarization-resolved Raman scattering experiments under high magnetic fields up to 31 T and temperatures down to ~0.5K. Highlights our recent results in high-field Raman magnetospectroscopy of quantum magnets will be presented with a specific focus on exploring the B-T phase diagram across the 1/3 magnetization plateau in spin-½ triangular-lattice antiferromagnet $K_2Co(SeO_3)_22$ and understanding anisotropy of magnetic interactions in a candidate quantum-spin-liquid material $Na_3Co_2SbO_6$.

Keywords: quantum magnets, spin excitations, magnons, spin-phonon coupling

[Abstract:0125] [Biology/Biomedicine]

Raman Spectroscopy for Detection of Tyrosine Kinase Inhibitor Resistance in Chronic Myelogenous Leukemia

***Sreeparna Nath*[1], *Arti Hole*[1], *Bhausaheb Bagal*[2], *Rukmini Govekar*[3], *Murali Krishna Chilakapati*[1]**

[1]*Chilakapati Lab, ACTREC-TMC, HBNI, Mumbai, India*
[2]*Adult Haematolymphoid Disease Management Group, Tata Memorial Centre, HBNI, Mumbai, India*
[3]*Rukmini Lab, ACTREC-TMC, HBNI, Mumbai, India*

Chronic Myelogenous Leukaemia (CML) is a myeloproliferative disorder characterized by the presence of Philadelphia chromosome, a shortened chromosome 22 resulting from a reciprocal chromosomal translocation between chromosome 9 and 22. Diagnostic indicators for CML include elevated myeloid cell numbers, the presence of immature myeloid cells in blood samples, and the detection of the translocation-derived transgene. The disease is initially controlled by tyrosine kinase inhibitors (TKIs), but if patients become unresponsive to TKIs, the disease progresses to the terminal stage of Blast Crisis. The reasons for resistance are diverse, and so are the methods used for its detection, making follow-up technically demanding and limiting its applicability in resource-poor countries with limited healthcare facilities. A single method capable of detecting resistance, irrespective of the underlying mechanism, would be beneficial in addressing this challenge.

Raman Spectroscopy captures the biochemical profile of a sample and requires minimal sample preparation. It has previously shown potential as a promising tool for detecting cancers and our previous study has also demonstrated its ability to differentiate between TKI-resistant and sensitive cell lines. In this study, spectral acquisitions were performed using a Raman microscope (WiTec alpha300R, Ulm, Germany) equipped with a 532 nm excitation laser operated at 8 mW at the sample and a 600 grooves/mm grating. Raman spectra were recorded with an acquisition time of 5 s and 10 accumulations and the interpolated fingerprint region of the spectra was extracted for subsequent multivariate analyses. Spectra were recorded from cell pellets, plasma and serum samples obtained from imatinib-sensitive CML patients and systematically compared with those from imatinib-resistant CML patients.

Multivariate analysis, employing Principal Component Analysis (PCA) and Principal Component–based Linear Discriminant Analysis (PC-LDA), yielded classification accuracies of 80% in cells, 75% in plasma, and 81.25% in serum. Furthermore, exploratory Multivariate Curve Resolution (MCR) was applied to the spectral data to elucidate molecular differences between the two groups. These findings indicate that RS has strong potential as a label-free approach for monitoring TKI resistance in CML and hold potential for broader application in larger patient cohorts and resource-limited healthcare environments.

Keywords: Chronic Myelogenous Leukaemia, Raman Spectroscopy, PCA, PC-LDA, MCR

[Abstract:0129] [Biology/Biomedicine]

Machine Learning and Data Science in IR Spectroscopy for Biomedical Applications

***Shuxia Guo*[1], *Pegah Dehbozorgi*[2], *Shweta Devani*[1], *Thomas Bocklitz*[1]**

[1]*Photonic Data Science, Leibniz Institute of Photonic Technology, 07745 Jena, Germany*
[2]*Institute of Physical Chemistry (IPC) and Abbe Center of Photonics (ACP), Friedrich Schiller University Jena, 07743 Jena, Germany*

In the last two decades, IR spectroscopy has received extensive attention due to their non-invasive and label-free detection in biological and biomedical investigations. IR spectroscopy detects and characterizes the molecular vibrations within a sample, based on the fact that a sample illuminated with IR light absorbs the light of the same frequency as its molecular vibrations. The intensity of the absorption is determined by the number of molecules and the absorption coefficients of the molecules. This supports to derive the molecular composition of a sample according to the (Bouguer)–Beer–Lambert (BBL) law and to conduct both quantitative and qualitative analysis.

The application of IR spectroscopy is indispensable with machine learning and data analysis, in which the spectroscopic signals are translated to knowledge under exploration, be it diagnosis or biological properties of a sample. Our research activities are centered around the development and applications of machine learning and deep learning models to leverage stable and reliable performance of such translation. In this presentation, we will report our latest results and methods on IR spectral analysis for biological applications, covering different steps of the full pipeline from pretreatment to model interpretation.

Acknowledgments

We highly acknowledge the project TELEGRAFT (101057673) with the funding from the European Union's 9th Framework Program Horizon Europe. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the Health and Digital Executive Agency. Neither the European Union nor the granting authority can be held responsible for them. This work is additionally supported by the BMBF, funding program Photonics Research Germany (LPI-BT1-FSU, FKZ: 13N15466; LPI-BT3-FSU, FKZ: 13N15710; LPI-BT4-Leibniz IPHT, FKZ: 13N15713) and is integrated into the Leibniz Center for Photonics in Infection Research (LPI).

Keywords: IR spectroscopy, Machine learning, Biomedical applications

[Abstract:0130] [Materials]

Optimisation of Through-Vial Raman Analysis of Turbid Samples by Modelling the Raman Intensity-Depth Decay Response

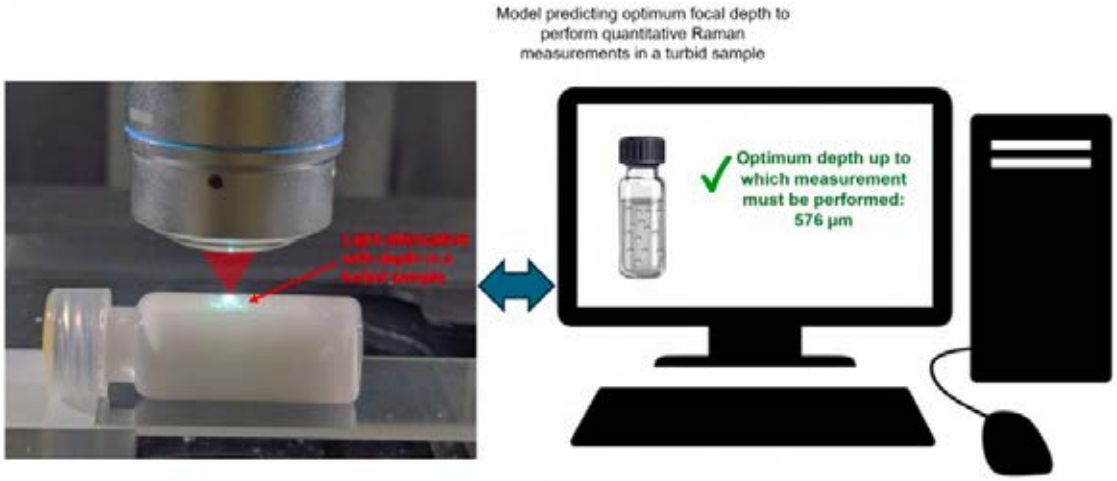
***Vasundhara Tyagi*[1], *Alex G Shard*[1], *Ryan T. Coones*[1], *Dimitrios Tsikritsis*[1], *Enya Murray*[1], *Elizabeth Legge*[1], *Caterina Minelli*[1], *Natalie Belsey*[1], *Natalie Belsey*[2]**

[1]*Chemical and Biological Sciences Department, National Physical Laboratory, Hampton Road, Teddington, Middlesex, TW11 0LW, UK.*
[2]*Department of Chemical & Process Engineering, University of Surrey, Guildford, GU2 7XH, UK.*

Raman spectroscopy enables non-destructive chemical analysis and can be performed through-vial, eliminating air exposure. However, signal attenuation arises from refraction, absorption, and scattering within the sample, while distortions and spectral interference from the vial further degrade signal collection and data quality. This study investigates depth-dependent Raman intensity decay in polystyrene (PS) particle suspensions as a model for turbid liquids and proposes a framework of equations and approaches based on Mie scattering theory and the Beer–Lambert law to predict Raman intensity decay in a range of samples. Experimental validation was performed using aqueous suspensions containing 495 nm, 350 nm, and 200 nm PS particles using an 830 nm laser, with Raman spectra acquired at incremental depths. Peak areas corresponding to PS, water, and glass were recorded. Mie theory was used to model the UV–visible extinction response, yielding estimated absorbance and, combined with the intensity decay due to refraction established from non-turbid samples, Raman intensity decay lengths. Estimated decay lengths for PS and water showed good agreement with experimental values, typically within 20 %. This framework enables rapid optimisation of focal depth and consistent comparison between samples and experiments for quantitative through-container Raman analysis in pharmaceuticals, materials science, and nanotechnology.

Keywords: raman modelling, through vial Raman, Raman for turbid samples

Graphical abstract



[Abstract:0131] [Coherent Raman Imaging]

Wide-Field Hyperspectral Coherent Anti-Stokes Raman Scattering (CARS) Microscopy Using Speckled Illumination

***Lilian Magermans*, Federico Vernuccio, Assia Benachir, Sandro Heuke, Anne Sentenac, Hervé Rigneault**

Aix Marseille Université, CNRS, Centrale Med, Institut Fresnel, Marseille, France

Rapid, label-free imaging over large fields of view is of high importance for many applications, including live-cell imaging and histology. Coherent Raman Scattering approaches such as coherent anti-Stokes Raman scattering (CARS) microscopy provide label-free chemical contrast but imaging large fields of view remains challenging. This is because conventional CARS microscopy is typically performed in a point-scanning configuration where tightly focused pump and Stokes beams are scanned across the sample. While this configuration provides intrinsic optical sectioning, it limits acquisition speed over extended areas and requires high peak intensities that may induce photo damage. In addition, the non-resonant background (NRB) inherent to CARS can distort spectral line shapes and reduces chemical specificity.

Here, we present a wide-field microscope able to overcome these issues by combining the advantages of random illumination microscopy (RIM) with those of hyperspectral CARS. In RIM, the sample is illuminated by a sequence of random speckle patterns and an optically sectioned, super-resolution image is reconstructed by applying computational algorithm to the speckled images. We have previously shown that RIM can be applied in the case of CARS microscopy by making both pump and Stokes beams speckled, and that such RIM-CARS has comparable optical sectioning to point-scanning CARS. However, this initial RIM-CARS demonstration was limited to samples with inherently low NRB. Here, we overcome the NRB by incorporating our recently developed tunable optical parametric amplifier laser system to acquire hyperspectral images by rapidly tuning the wavelength of the pump beam. A phase-retrieval algorithm is then applied to the recorded spectra, which allows to remove the NRB and restore the chemical sensitivity of CARS.

The resulting hyperspectral RIM-CARS microscope is able to perform label-free chemical imaging over fields of view of 200-by-200 μm with optical sectioning and super resolution, which we demonstrate on various test- and biological samples.

Keywords: CARS Microscopy, Hyperspectral Imaging, Speckle illumination, Random Illumination Microscopy

[Abstract:0134] [SERS/TERS/Plasmonics]

In-Solution SERS for Liquid Biopsies Using a Portable Raman Device for Point-of-Care Testing

***Ahmed Y. F. Mahmoud*[1], *Sandra M. Guerrero Pattugalan*[2], *Rawan Almasri*[3], *Lorraine O'Driscoll*[3], *Aidan D. Meade*[1], *Fiona M. Lyng*[1]**

[1]*Radiation and Environmental Science Centre, Physical to Life Sciences Research Hub, FOCAS Building, Technological University Dublin, Aungier Street, D02 HW71 Dublin, Ireland and School of Physics, Clinical and Optometric Sciences, Technological University Dublin, Central Quad, City Campus, Grangegorman D07 XT95, Dublin, Ireland*
[2]*Faculty of Experimental Science, Universidad Francisco de Vitoria, Madrid, Spain*
[3]*School of Pharmacy and Pharmaceutical Sciences, Trinity Biomedical Sciences Institute, & Trinity St. James's Cancer Institute, Trinity College Dublin, Dublin, Ireland*

Surface-enhanced Raman scattering (SERS) has been shown to be a powerful analytical technique capable of single-molecule detection. In addition, SERS applications have been expanding significantly in liquid biopsy with the advent of handheld and portable Raman spectrometers. Although these portable devices can enable field deployment and minimal sample preparation at the point of need, they come with technical limitations in controlling laser focusing, power, and acquisition time that can hinder their full analytical potential. One way to circumvent these limitations is to systemically optimize the in-solution SERS substrate performance to accompany these devices. Among many types and shapes of plasmonic nanostructures, gold nanostars (AUNs) have demonstrated their potential as in-solution SERS substrates, owing to the tunability of their surface plasmon resonance over a wide wavelength range and their high electromagnetic enhancement at the tips of their branches.

In this talk, we present a systematic study of Good's buffer gold nanostars (AUNs) as in-solution SERS substrates via the formation of metal-liquid-like films (MELLFs) at the liquid-liquid interface using a portable Raman device. AUNs plasmonic behavior and morphology were characterized by different techniques, such as, extinction spectroscopy, dynamic light scattering, and electron microscopy. We will discuss how different experimental parameters, such as the concentration of AUNs and the type of promoters used for self-assembly, can influence the MELLF formation and, in turn, the SERS performance. A systematic comparison of the SERS performance of the MELLFs approach against the most commonly used approach of salt aggregation will be demonstrated, using different molecules, such as, Raman reporters, DNA, and extracellular vesicles (EVs). SERS spectral profiling of EVs can offer a unique means of differentiating between healthy and disease states. Pros and cons of each approach will be discussed in terms of SERS enhancement, reproducibility, stability, and ease of use. Integrating in-solution SERS, portable Raman devices, and liquid biopsy can provide numerous opportunities for SERS biosensing platforms to be utilized at the point-of-care.

Keywords: SERS, SERS substrate, liquid-liquid interface, portable Raman, and liquid biopsy

Oral Abstracts

[Abstract:0135] [Non-linear/Time-resolved]

Ultrafast Charge Transfer Dynamics Probe by Time-Resolved Raman Spectroscopy

Jongwon Im, Sebok Lee, Yoonsoo Pang

Department of Chemistry, Gwangju Institute of Science and Technology, Gwangju, Republic of Korea

Intramolecular charge transfer (ICT) has garnered significant interest in chemistry and related fields due to its extensive applications. The structural changes of chromophores upon ICT may lead to dramatic changes in photophysical properties, including emission quantum yields. Recently, we demonstrated that skeletal vibrations of push-pull chromophores obtained from femtosecond stimulated Raman spectroscopy (FSRS) can sensitively probe the structural changes of p-conjugated backbones (stilbene, biphenyl, and styrylpyran) upon the ICT in the excited states. In this work, we report the ICT dynamics of thioflavin T (ThT) and stilbazolium derivatives obtained from FSRS and impulsive stimulated Raman spectroscopy (ISRS).

ThT is a well-known fluorophore used to visualize amyloid fibrils associated with Alzheimer's disease. In polar solvents, efficient ICT quenches ThT's fluorescence, while binding to amyloid fibrils inhibits the ICT, resulting in strong fluorescence. We investigated the ICT dynamics of ThT using ISRS and FSRS. The skeleton modes (1500-1600 cm-1) from FSRS and the low-frequency vibrational modes (200-650 cm-1) from ISRS revealed two ICT dynamics in aliphatic alcohol solutions (~370 fs and 3.4 ps in 1-butanol). Theoretical calculations by time-dependent density functional theory suggest multifaceted structural changes of ThT during ICT, where the bending of benzothiazole group (~370 fs) is followed by the twisting of dimethylaniline (3.4 ps) group.

We also examined para- and ortho-substituted stilbazolium derivatives (p-DEST and o-DEST), which show similar ICT lifetimes (~0.7 ps) in transient absorption (TA) measurements but distinct vibrational signatures in FSRS. Notably, the strong ν8a band at 1650 cm^{-1} in p-DEST indicates diethylaniline twisting, absent in o-DEST. Further studies with N-methylpyridinium isomers, designed to restrict rotational freedom, underscore the importance of vibrational probes in capturing ultrafast structural changes during ICT. These findings highlight the nuanced interplay between molecular structure and ICT dynamics, offering deeper insight into the excited-state behavior of push-pull chromophores.

Keywords: intramolecular charge transfer, push-pull chromophores, stimulated Raman, transient absorption

[Abstract:0136] [Biology/Biomedicine]

Multimodal Raman and Infrared O-PTIR Spectroscopy for Detection of Transforming Hr-HPV Infection in Single Cervical Cells

***Muhammad Asyraf Onn*[1], *Rubina Shaikh*[2], *Cara Martin*[3], *John O' Leary*[4], *Hana Mc Mahon*[5], *Kate Cuschieri*[5], *Mustafa Kansiz*[6], *Cassio Lima*[7], *Royston Goodacre*[7], *Fiona Lyng*[1]**

[1]*Radiation and Environmental Science Centre (RESC), Physical to Life Sciences Research Hub, Technological University Dublin (TU Dublin), Ireland*
[2]*School of Physics, Clinical and Optometric Sciences, Grangegorman Campus, Technological University Dublin (TU Dublin), Ireland*
[3]*Trinity College Dublin (TCD) CERVIVA Molecular Pathology Laboratory, The Coombe Hospital, Ireland*
[4]*Discipline of Histopathology, School of Medicine, Trinity Translational Medicine Institute (TTMI), Trinity College Dublin, Ireland*
[5]*Scottish HPV Reference Laboratory, Department of Laboratory Medicine, NHS Lothian, 51 Little France Crescent, Edinburgh EH16 5SA, Scotland, UK*
[6]*Photothermal Spectroscopy Corporation, Santa Barbara, California 93111, USA*
[7]*Centre for Metabolomics Research, Department of Biochemistry, Cell and Systems Biology, Institute of Systems, Molecular and Integrative Biology, University of Liverpool, Liverpool, UK*

Cervical cancer remains a significant global health challenge, ranking as the eighth most common cancer worldwide with approximately 662,301 new cases annually [1]. This burden persists despite the widespread implementation of HPV vaccination and primary HPV-based screening programmes. A critical unmet clinical need is the objective identification of transforming high-risk HPV (hr-HPV) infections, particularly distinguishing transcriptionally active (HPV DNA+/mRNA+) cases from transient infections (HPV DNA+/mRNA-). Previous studies using Raman spectroscopy on ThinPrep cervical cytology samples demonstrated high sensitivity and specificity for detecting high-grade cytological abnormalities and differentiating HPV infection states [2],[3]. Here, we extend single-cell Raman analysis using optical photothermal infrared (O-PTIR) microscopy, enabling simultaneous acquisition of Raman and infrared (IR) spectra from identical submicron cellular locations. Raman and IR spectra were recorded from cervical exfoliated cell ThinPrep samples from four clinically defined groups (cytology normal HPV DNA-/mRNA-, cytology normal HPV DNA+/mRNA-, cytology abnormal HPV DNA+/mRNA- and cytology abnormal HPV DNA+/mRNA+). Mean IR and Raman spectra demonstrate reproducible multimodal signatures across each of the four groups. Key Raman discriminative features include bands at ~752, 785, 1095 cm^{-1} (DNA/RNA backbone), 1000 cm^{-1} (phenylalanine), 1240 - 1265 cm^{-1} (amide III), 1445 cm^{-1} (lipids/proteins), and 1655 cm^{-1} (amide I). Complementary IR bands were observed at ~1650 cm^{-1} (amide I), ~1545 cm^{-1} (amide II), ~1400 – 1450 cm^{-1} (lipids/proteins) and ~1240 cm^{-1} (nucleic acids), providing additional biochemical information to the molecular signatures. Spectra from the HPV DNA+/mRNA+ group (transforming HPV infection) exhibit enhanced nucleic acid-associated intensity and altered protein/lipid ratios, consistent with increased transcriptional activity. Spectral datasets will be used to develop supervised classification models to identify transforming HPV infection. The integration of complementary vibrational modalities from identical cellular regions reduces spatial heterogeneity and enhances biomarker robustness. This study demonstrates the feasibility of multimodal O-PTIR vibrational spectroscopy for single-cell cervical cytopathology and the detection of transforming HPV infections. The technique shows promise for distinguishing transient from clinically significant infections, although further studies are required to validate its diagnostic performance. Such an approach may contribute to global cervical cancer elimination efforts by improving the identification of clinically relevant transforming HPV infections.

Keywords: O-PTIR spectroscopy, Raman spectroscopy, Multimodal, HPV, Cytopathology, Cervical cancer

Oral Abstracts

[Abstract:0139] [Theory/Computation]

Why Do Raman Features Change with Excitation Wavelength? How Resonance States Shape Raman Spectra

***Giacomo D'Arcangelo*[1,2], *Julien Bloino*[1]**

[1]*Scuola Normale Superiore, Piazza dei Cavalieri 7, Pisa, Italy, 56126*
[2]*Applied and Laser Spectroscopy Laboratory, Institute of Chemistry of Organometallic Compounds, Research Area of National Research Council, Via G. Moruzzi, 1, Pisa, Italy, 56124*

Besides providing detailed molecular-structure information, Raman spectroscopy can, under specific conditions, become an indirect probe of excited-state properties in molecular systems, offering insight into excited-state dynamics often relevant to natural processes. Under electronic-resonance conditions, selective investigation of specific electronic states becomes feasible by fine-tuning the incident excitation energy. In this regime, the scattering amplitudes are mediated by intermediate vibronic levels; therefore, the strongly reshaped Raman intensities encode ground–excited-state vibrational interactions, going beyond a purely ground-state picture.

In this contribution, we highlight the critical role of theoretical tools not only for the prediction of Raman spectral patterns, but also for the interpretation and simulation of Raman Excitation Profiles (REPs), which track the intensity variations of individual vibrational modes as a function of the excitation energy and provide direct insight into vibronic coupling effects. (see Fig.1)

The complexity of resonance Raman signals poses challenges from both experimental and theoretical perspectives; experimentally, the main challenge in the study of the lowest excited state is fluorescence, because excitation and scattered light often fall within the spectral range of the most probable fluorescence emission (Kasha's rule).

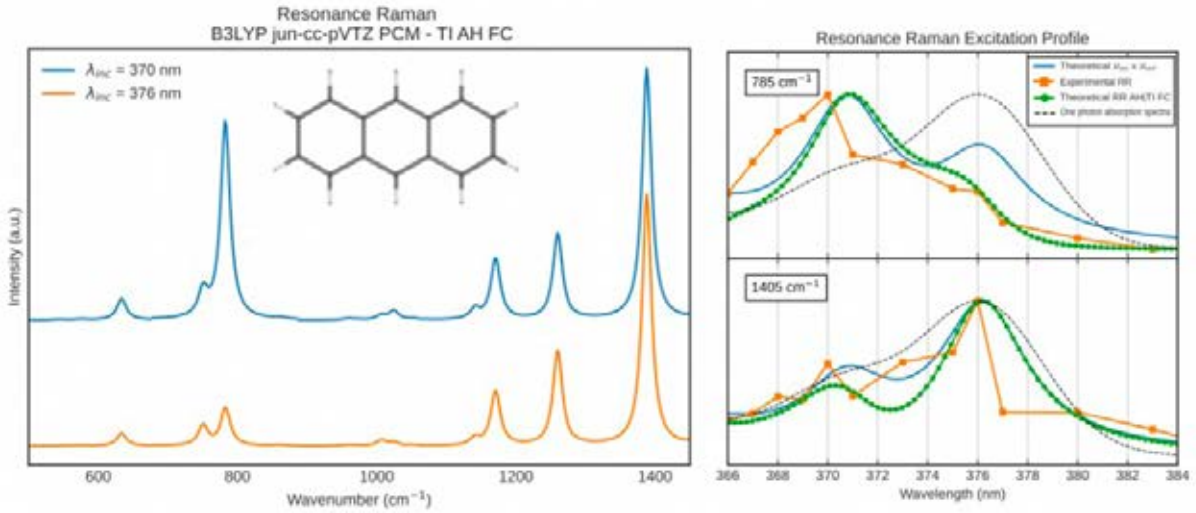
Advanced techniques such as time-resolved methods exploiting the distinct signatures of scattering and fluorescence processes (e.g. Kerr-gated Raman spectroscopy) enable the acquisition of high-quality spectra and improved spectral resolution even in the resonance regime.

Recently, such approaches have been used to probe how Raman intensities depend on excitation energy for anthracene, via scans in the 366–386 nm, demonstrating how laser energy modulates Raman bands under electronic resonance in a representative case study. [J. Phys. Chem. Lett. 2025, 16, 39, 10180–10186]

From the theoretical perspective, we discuss key computational challenges in modeling resonant Raman scattering and emphasize the need for validation through a tight experiment–theory interplay, which is essential to resolve open questions in electronic structure (e.g. TD-DFT) and vibronic modeling and to obtain a realistic picture of vibronic–electronic resonances explored by the Raman technique. We also present Franck–Condon-based computations to dissect the individual contributions governing Raman intensities under resonance conditions, enabling a detailed analysis and fast prediction of the ground–intermediate-state interactions that shape the Raman response.

Keywords: Resonance Raman, Vibronic Coupling, Electronic resonances, DFT Spectroscopy

Resonance Raman spectra and excitation profiles of anthracene



Resonance Raman spectra and Raman excitation profiles (REPs) for anthracene. Left: simulated resonance Raman spectra at two incident wavelengths (λ_inc = 370 and 376 nm) at the B3LYP/jun-cc-pVTZ level of theory with PCM within the TI-AH-FC vibronic framework. Right: comparison between experiment and theory (and product of transition probabilities |μim| × |μmf|) for the REPs of the 785 cm^{-1} and 1405 cm^{-1} modes over the 366–384 nm window; the dashed trace reports the one-photon absorption profile to highlight the resonance region.

[Abstract:0142] [Novel Approaches]

Multimodal Characterisation of Li-Based Battery Materials Using In Situ Raman and SEM Analysis

***Jorge Diniz*[1], *Jennifer Ferguson*[1], *Ryuichi Kato*[2]**

[1]*Renishaw PLC, Wotton-under-Edge, UK*
[2]*Renishaw KK, Tokyo, Japan*

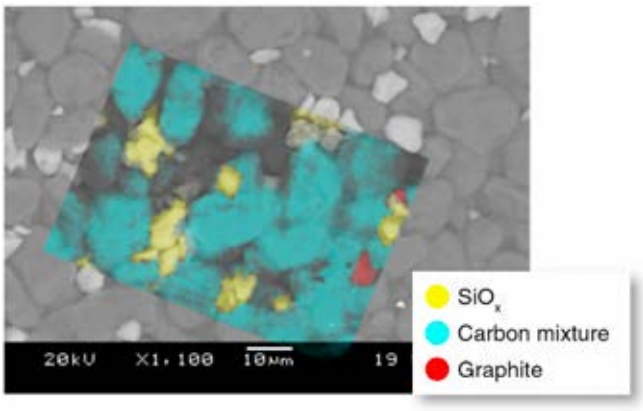
Lithium-ion (Li-ion) batteries are widely used as energy storage devices. The high demand for energy storage solutions and the decrease in fossil-fuel dependency has driven the need to improve the performance, safety and lifetime of such systems. The properties of Li-ion batteries are governed by multiscale phenomena such as porosity, particle fracture, binder homogeneity and interphase transformations during de/sorption of Li ions, to name a few. Therefore, understanding the link between morphology and chemistry across length scales can lead to the fabrication of more durable, stable and higher capacity battery systems.

Multimodal, correlative imaging approaches can co-register the structural and spectroscopic information for enhanced understanding of batteries. For example, SEM (scanning electron microscopy) provides highresolution information into particle size/element distribution, morphology, porosity, and interfacial properties, while Raman spectroscopy provides nondestructive identification of polymorphs, quantifies carbon quality (D/G bands), detects stress and local bonding environments, and probes the state of lithium and metal oxide species. However, performing both analyses in the same regions when using separate instruments is challenging. Furthermore, the active materials are susceptible to degradation when exposed to the atmosphere, requiring specialised sample transferring between instruments.

Here, we present results showing the benefits of integrating Raman spectroscopy into a SEM microscope, enabling colocalised and simultaneous Raman and SEM imaging without the need to move or transfer the sample. We demonstrate how Raman can give insights to the identification and distribution of carbon structures (graphitic/amorphous) and to Li desorbing processes and how those correlate with crystal orientation or morphology. This approach will enable the acceleration of Liion battery materials optimisation.

Keywords: correlative Raman imaging, Raman in-SEM, battery materials

Battery anode



Correlative SEM and Raman images of a carbon-coated battery anode illustrating the distribution of different forms of carbon and silicon.

[Abstract:0143] [Biology/Biomedicine]

Serum Raman Spectroscopy for Oral Disease Stratification

***Panchali Saha*[1], *Poonam Joshi*[3], *Arti Hole*[2], *Pankaj Chaturvedi*[3], *Murali Krishna Chilakapati*[1]**

[1]*Chilakapati Laboratory Tata Memorial Centre, Advanced Centre for Treatment, Education and Research in Cancer (TMC-ACTREC) Kharghar Navi Mumbai, Maharashtra, India, Training School Complex, Homi Bhabha National Institute, Anushakti Nagar, Maharashtra, India*
[2]*Chilakapati Laboratory Tata Memorial Centre, Advanced Centre for Treatment, Education and Research in Cancer (TMC-ACTREC)Kharghar Navi Mumbai, Maharashtra, India,*
[3]*Tata Memorial Centre, Advanced Centre for Treatment, Education and Research in Cancer (TMC-ACTREC)*

Oral cancer remains a serious health concern, particularly in India, where patient outcomes are often limited by late detection. Lesions that precede invasive oral cancers often appear benign, resulting in patients presenting to clinics in advanced stages.Despite advances in treatment modalities, overall survival rates have shown little improvement in recent decades, with the global 5-year survival rate remaining around 50%. The major contributors to poor prognosis are delayed detection and disease relapse, which is strongly associated with reduced survival. Development of improved strategies for early detection and monitoring are therefore, essential. Minimally invasive approaches that can capture biochemical alterations are of considerable interest for improving detection and prognostic evaluation. In this context, Raman spectroscopy, has emerged as a promising tool for biomedical analysis. In the present study, blood serum-based Raman spectroscopy was explored to investigate biochemical variations associated with oral disease. Blood samples were obtained from individuals representing different clinical categories of oral health and disease, including patients being treated for oral cancer. Serum samples were subjected to Raman spectroscopy. Raman spectral datasets were used to construct classification models using multivariate approaches to distinguish between clinically defined groups. Results indicated that serum Raman spectra contain detectable molecular information reflecting biochemical variations across the studied cohort. Classification models derived from the spectral data demonstrated encouraging performance, with an overall identification accuracy as high as 100% for certain groups. These findings highlight the potential of minimally invasive serum-based Raman spectroscopy for rapid identification and monitoring of oral diseases.

Keywords: Oral cancer, Raman spectroscopy, blood

[Abstract:0146] [Novel Approaches]

Novel Raman Sensor for High-Resolution Detection of Small Spectral Shifts

***Katarzyna Szykula Meurs*[1], *Oliver Lischtschenko*[2], *Martin Jaeger*[3], *Maarten Honing*[1]**

[1]*M4i Institute, Faculty Health, Medicine & Life Sciences Maastricht University, Universiteitssingel 50, 6229 ER Maastricht, the Netherlands*
[2]*Coher Sense UG, im Technikzentrum Lübeck, Maria-Goeppert-Str. 1, 23562 Lübeck, Germany*
[3]*Department of Chemistry and ILOC, Niederrhein University of Applied Sciences, Frankenring 20, 47798 Krefeld, Germany*

Detecting extremely small spectral shifts in Raman bands remains a fundamental challenge for conventional Raman spectroscopy. While modern spectrometers provide high spectral resolution, their practical spectral accuracy and stability often limit the reliable detection of sub–wavenumber band position changes. Such minute shifts, however, frequently carry critical chemical information, particularly in processes where structural changes occur gradually.

In this work, we present a novel Raman sensing concept designed specifically for the detection of extremely small Raman band shifts. The approach focuses on achieving ultra-high spectral accuracy, enabling the detection of subtle changes in Raman band positions that are typically inaccessible with conventional Raman instrumentation.

To demonstrate the potential of this approach, oxidation processes in unsaturated fatty acids were investigated as a model system. Oxidation leads to subtle modifications of vibrational modes associated with the C=C bond, producing very small band shifts that appear well before significant spectral changes or degradation products become observable with standard Raman spectroscopy. The proposed sensing concept enables the detection of these early-stage transformations, acting as a “first-response” monitoring tool.

Beyond lipid oxidation studies, this novel Raman sensing strategy offers a promising pathway for applications requiring highly sensitive detection of spectral shifts, including process monitoring within Process Analytical Technology (PAT) environments.

Keywords: Raman sensor, spectral shift, fatty acids, oxidation, PAT

[Abstract:0147] [Industrial/Societal Applications]

Fluorescence Suppression Techniques for Through-Container Raman Spectroscopy

***Ané Kritzinger*[1], *Admir Bajraktarevic*[1], *Ralf Mouthaan*[1], *George O. Dwapanyin*[2], *Graham D. Bruce*[2], *Kishan Dholakia*[1]**

[1]*Centre of Light for Life and School of Biological Sciences, The University of Adelaide, Adelaide, Australia*
[2]*SUPA, School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, Fife, UK*

The non-contact nature of Raman spectroscopy makes it suitable for non-destructive and non-invasive molecular analysis. However, its ability to directly analyse packaged products is severely hindered by strong fluorescence signals originating from the container wall, which overwhelms the Raman signal of the contents. Additionally, absorption by the container of both the excitation laser and Raman signal further decreases the already weak Raman signal. Here, we present three fluorescence suppression techniques — wavefront shaping, wavelength modulation, and time-gating — each operating in a different domain (spatial, spectral, and temporal) to isolate the Raman signal of the contents from fluorescence interference.

First, we employ wavefront shaping using an axicon lens to spatially reject the container signal. The conical excitation beam forms an annulus on the container wall before collapsing to a focus inside. Raman light, excited at the focus, is collected through the central dark region, making it spatially separate from the container's signal while maintaining co-linearity between the excitation and collection paths, effectively suppressing container fluorescence.

Second, we apply wavelength-modulated Raman spectroscopy (WMRS) to further suppress fluorescence and enhance the Raman signal. By tuning the excitation wavelength over a small range (<2nm), Raman peaks shift spectrally with the excitation wavelength while fluorescence remains stationary, allowing their separation and providing an inherent baseline correction without artefacts due to fitting.

Third, we explore time-gated Raman spectroscopy as a temporal approach to fluorescence rejection. By time-gating the detector to a narrow window following the excitation pulse, the fluorescence is rejected while the near-instantaneous Raman signal is captured.

Combining wavefront shaping and WMRS, we demonstrate methanol quantification in sealed spirit bottles, achieving a signal-to-noise ratio enhancement of up to 12 times and a limit of detection of 0.2% v/v in 40% v/v ethanol, ten times below the safety threshold, validated through coloured glass bottles and on a real commercial spirit sample.

By addressing fluorescence interference spatially, spectrally, and temporally, these three approaches offer independent or combined deployment for non-invasive sensing. While demonstrated here for methanol safety screening, these techniques are broadly applicable to analysis of any packaged product where container interference limits Raman measurement.

Keywords: Wavefront shaping, wavelength modulation, time-gating, through-container, non-invasive, methanol quantification

[Abstract:0148] [SERS/TERS/Plasmonics]

Selective SERS Detection of Nerve Agents Using Oxime-Based Raman Probe Molecules

***Rasmus Öberg*[1], *Nora Molander*[1], *Damir Asoli*[3], *Magnus Engqvist*[1], *Magnus Andersson*[2], *Tomas Rindzevičius*[4], *Anja Boisen*[4], *Andreas Larsson*[1], *Per Ola Andersson*[1]**

[1]*Swedish Defence Research Agency (FOI), Umeå, Sweden*
[2]*Department of Physics, Umeå University, Umeå, Sweden*
[3]*Silmeco ApS, Copenhagen, Denmark*
[4]*Department of Health Technology, Technical University of Denmark, Copenhagen, Denmark*

Nerve agents are a group of organophosphate chemicals classed as chemical warfare agents. As they are both highly lethal, and difficult to detect in small amounts, the development of effective sensing methods for nerve agents is a pressing security concern. To address this concern, plasmonic techniques such as surface-enhanced Raman spectroscopy (SERS) have shown promise for rapid and highly selective sensing of many harmful substances. However, the application of SERS to nerve agents has so far been limited by their inherently poor Raman scattering cross-section, as well as limited research into the field caused by limitations in working with these agents.

Here, we will present our work in developing a novel and custom-designed Raman probe molecule: 4-Thiophene Pyridine Amido Oxime (TPAO), which enables selective and sensitive sensing of live nerve agents in liquid media, even using portable Raman instruments with limited spectral resolution. We report a detection limit of the traditionally difficult-to-detect nerve agent Cyclosarin of downward 1 ppm, a factor 100 improvement over previous works. Furthermore, we use principal component analysis to demonstrate how TPAO-assisted SERS can be used to separate between chemically similar nerve agent molecules and other less lethal organophosphates (e.g. pesticides and flame retardants). Lastly, we demonstrate the robustness of TPAO, as it is used to detect nerve agents in complex backgrounds. Altogether, this work represents a significant step toward achieving rapid and selective field detection of live nerve agents using SERS.

Keywords: Sensing, Nerve Agents, TPAO, VX, Tabun, Cyclosarin

[Abstract:0151] [Theory/Computation]

Atomic Contributions to the Raman Intensity Reveal Molecular Charge Density Shifts – a Combined Experimental and Computational Approach

***Marc Bröckel*[1], *Johannes Gierschner*[2], *Alfred Meixner*[1], *Kai Braun*[1]**

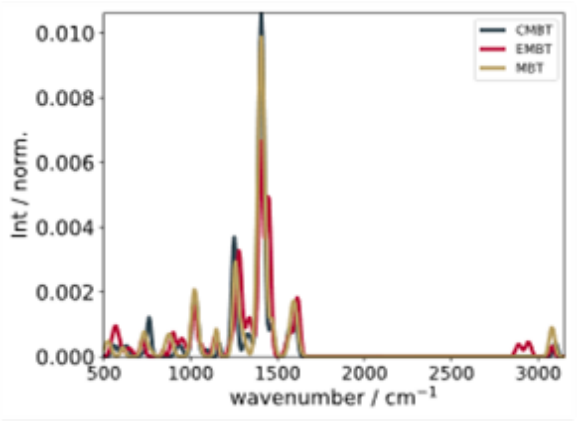
[1]*Eberhard Karls Universität Tübingen, Institute of Physical and Theoretical Chemistry, Tübingen, Germany*
[2]*Madrid Institute for Advanced Studies, IMDEA Nanoscience, Madrid, Spain*

Understanding the molecular electron density, a fundamental property governing molecular interactions, plays a vital role in determining molecular structures, bonding patterns, and overall chemical reactivity. This knowledge is crucial for e.g. designing molecules with tailored properties in fields such as pharmacology, materials science, or organic optoelectronics. Recently, we have shown via tip-enhanced Raman spectroscopy that a positive bias voltage applied to a gold tip in proximity to a molecule on a gold surface leads to a reversible electron density shift from the Au-substrate to the molecule observed as intensity increase in the corresponding TERS-spectra.

In this study, we employ surface-enhanced Raman spectroscopy (SERS) to probe the electron density of molecules from the 2-mercaptobenzothiazole (MBT) family. Introducing an ethoxy group (EMBT) or a chlorine atom (CMBT) drastically changes the molecular electron density which can be directly observed in the SERS intensity as shown in Figure 1. We present a method with which it is possible to partition the total Raman intensity into atomic contributions (Figure 2). Combining such "atomic Raman spectra" with visualizing the charge density oscillations that occur during a normal mode cycle yields a deep understanding of the Raman intensity and allows for experimental tracking charge density shifts with atomic resolution.

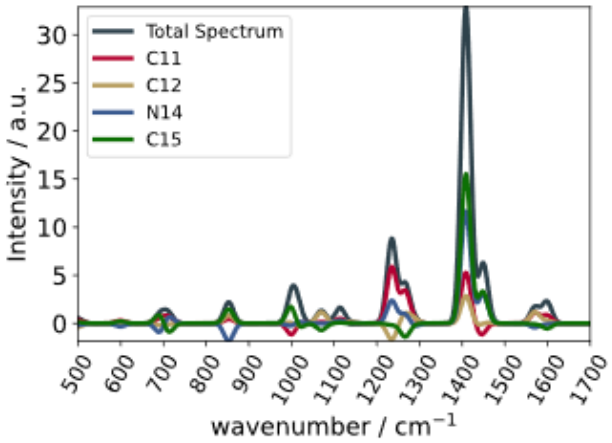
Keywords: Atomic Raman Intensities, SERS Computations, Charge Density Shifts

Figure 1



SERS Spectra of CMBT, EMBT and MBT. The peak intensities differ due to the different substituents

Figure 2



Calculated total SERS spectrum of MBT and the atomic contributions of atoms C11, C12, N14 and C15

Oral Abstracts

[Abstract:0152] [Biology/Biomedicine]

Raman Spectroscopic Analysis of Nanoparticle Uptake Dynamics in Human Cells

***Karolina M. Turczyńska*[1], *Faustyna Pachacz*[1], *Jakub Firlej*[1], *Malgorzata Baranska*[1], *Hugh J. Byrne*[2]**

[1]*Department of Chemical Physics, Faculty of Chemistry, Jagiellonian University, Krakow, Poland*
[2]*Physical to Life Sciences Research Hub, TU Dublin, Ireland*

Global plastic production and degradation have led to the widespread presence of micro- and nanoplastics in the environment, with emerging evidence linking exposure to cardiovascular dysfunction. However, the specific cellular mechanisms, particularly the kinetics of penetration and accumulation, remain poorly characterized at the subcellular level. Current research predominantly focuses on end-point toxicity (e.g. oxidative stress and cell death), leaving a gap in our understanding of the time-resolved nanoparticle internalization and trafficking.

In this study, we investigated the spatiotemporal dynamics of polystyrene nanoparticle interactions within human aortic endothelial cells (HAEC). Cells were exposed to carboxylated polystyrene nanoparticles across a series of time points to map uptake evolution. We employed label-free Raman hyperspectral imaging to detect and localize nanoparticles within complex cellular environments. This approach circumvents the need for external fluorescent labels, thereby preserving the native biological state and avoiding potential artifacts associated with dye-leaching or altered surface chemistry.

The integration of hyperspectral data with advanced multivariate modeling allowed for the precise quantification of nanoparticle distribution over time. These results provide a quantitative foundation that ultimately contributes to a deeper understanding of the mechanisms of environmental plastic exposure and informs the development of more effective targeted drug delivery systems.

This research was funded by the National Science Center Poland (NCN), OPUS 2024/53/B/ST4/02698 to Malgorzata Baranska.

Keywords: Raman mapping, nanoparticle uptake, spatiotemporal dynamics, nanoplastics

[Abstract:0187] [SERS/TERS/Plasmonics]

PEDOT:PSS Conducting Polymer Substrates: A Robust Platform For Highly Sensitive Surface-Enhanced Raman Scattering (SERS) Spectroscopy

***Marek Procházka*[1], *Eva Kočišová*[1], *Pavol Pivko*[2], *Daniil Nikitin*[2], *Jan Prokeš*[2], *Jan Hanuš*[2], *Ondřej Kylián*[2]**

[1]*Charles University, Faculty of Mathematics and Physics, Institute of Physics, Prague 2, Czech Republic*
[2]*Charles University, Faculty of Mathematics and Physics, Department of Macromolecular Physics, Prague 8, Czech Republic*

Sensitive, reproducible, and cost-effective substrates are essential for reliable surface-enhanced Raman scattering (SERS) detection. π-conjugated conducting polymers have recently emerged as promising non-plasmonic alternatives due to their tunable electronic structure and delocalized molecular orbitals. Here, we investigate spin-coated and thermally cured poly(3,4-ethylenedioxythiophene)-poly(styrenesulfonate) (PEDOT:PSS) films as robust SERS platforms, focusing on optimizing film preparation, thermal treatment, and analyte deposition.

PEDOT:PSS films were deposited on Si wafers and annealed at temperatures up to 350 °C and characterized by AFM, XPS, and resistance measurements. The results indicate that curing at 150 °C provides an optimal balance between PEDOT chain rearrangement and conductivity, while avoiding PSS degradation, and promotes effective charge transfer transitions between the HOMO of PEDOT:PSS and the LUMO of methylene blue (MB), the model analyte.

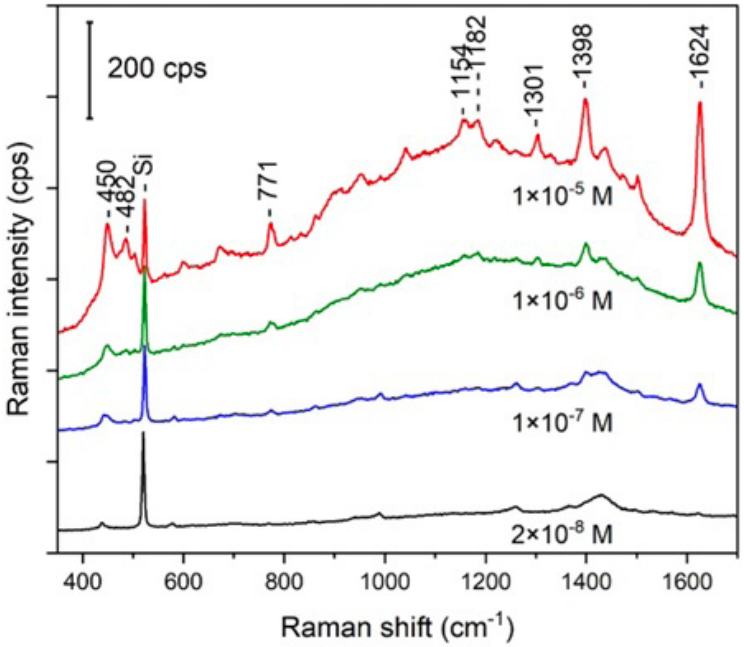
Two analyte deposition protocols were tested for SERS: (i) direct dropping and (ii) immersion for two hours. Immersion significantly improved SERS signals, yielding intensities approximately five times higher than dropping. Under these optimized conditions, PEDOT:PSS substrates enabled detection of MB down to 2×10^{-8} M (see Figure 1). SERS mapping across 20 × 20 spectral points with an increment of 5 μm revealed high spectral reproducibility with RSD of 1.8%. We also deposited PEDOT:PSS on paper and successfully detected 1×10^{-6} M MB.

Our results confirm that PEDOT:PSS films combine high SERS sensitivity with excellent spectral reproducibility, positioning them as a competitive, low-cost alternative to conventional noble metal and semiconductor-based substrates. Paper-based substrates offer several advantages, including low cost, ease of preparation, flexibility, and biocompatibility.

This work was supported by the grant 24-12197S from the Czech Science Foundation.

Keywords: surface-enhanced, SERS, charge transfer, conducting polymer, PEDOT:PSS

Figure 1. SERS spectra of MB measured from the PEDOT:PSS substrate immersed to various MB solution concentrations for two hours.



Oral Abstracts

[Abstract:0190] [SERS/TERS/Plasmonics]

Structural Characterization of Tel24 on Silver And Gold Nanoparticles Using SERS Spectroscopy

***Adriana Kenđel*, Klara Popović, Petra Petrović Popović, Snezana Miljanic**

Department of Chemistry, University of Zagreb Faculty of Science, Zagreb, Croatia

G-quadruplexes (G4s) are non-canonical secondary structures of nucleic acids formed by guanine-rich sequences. In living cells, they are involved in a range of essential biological processes. Considerable attention has been devoted to their role in telomere biology. The G-rich 3′ overhang of telomeres, composed of tandem TTAGGG repeats, can adopt G-quadruplex conformations that inhibit telomerase activity - an enzyme overexpressed in numerous cancer types and critically implicated in the uncontrolled proliferation of malignant cells. Accordingly, there is a clear need for analytical approaches capable of detecting and characterizing structural changes in G-quadruplexes under aqueous conditions that closely resemble the physiological environment, thereby facilitating a more comprehensive understanding of their mechanism of action. Surface-enhanced Raman scattering (SERS) spectroscopy is a highly sensitive vibrational spectroscopic technique that enables structural characterization of low-concentration analytes in the vicinity of nanostructured metal surfaces. Due to its high sensitivity and its ability to provide molecularly specific fingerprint spectra in aqueous media, SERS is particularly well suited for bioanalytical applications. To assess the suitability of SERS for the structural characterization of oligonucleotides capable of forming G4 structures, silver and gold colloidal nanoparticles were employed as metallic substrates. The nanoparticles were synthesized by chemical reduction of metal salts with sodium citrate. Subsequently, one portion of the prepared colloids was aggregated with magnesium sulfate, while the other was functionalized with thiol-modified telomeric DNA sequence d[$(TTAGGG)_4$] (Tel24). All SERS measurements for the Tel24 oligonucleotide were performed using 785 nm excitation. SERS spectra of Tel24 recorded on freshly prepared and aggregated nanoparticles were compared with spectra obtained from oligonucleotides-functionalized metal nanoparticles. Detailed analysis of band positions and relative intensities in the recorded SERS spectra demonstrated that surface modification of colloidal silver and gold nanoparticles significantly affects the stacking and orientation of the oligonucleotide at the metal surface. Aggregation of silver nanoparticles resulted in localized electromagnetic “hot spots” associated with enhanced inelastic scattering, providing the most suitable substrate for structural characterization of the Tel24 oligonucleotide.

Keywords: colloids, SERS, Tel24, G-quadruplexes

[Abstract:0193] [SERS/TERS/Plasmonics]

Photocatalytically Recyclable Nb_2O_5/Metal Hybrid Platforms For Surface-Enhanced Raman Scattering (SERS) Spectroscopy

***Eva Kočišová*[1], *Max Pavlović*[2], *Jan Hanuš*[2], *Marek Procházka*[1], *Ondřej Kylián*[2]**

[1]*Charles University, Faculty of Mathematics and Physics, Institute of Physics, Prague 2, Czech Republic*
[2]*Charles University, Faculty of Mathematics and Physics, Department of Macromolecular Physics, Prague 8, Czech Republic*

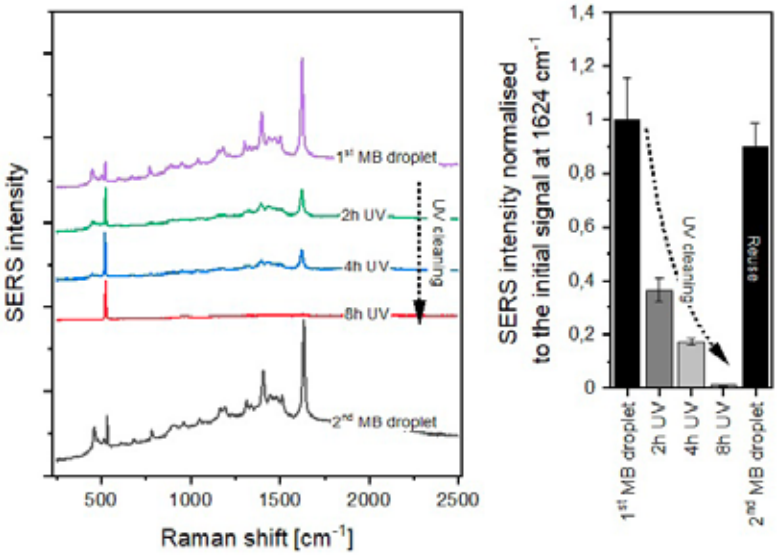
Metal–oxide/metal hybrid nanomaterials have attracted significant attention due to their unique physicochemical properties. One promising application is their use as recyclable platforms for surface-enhanced Raman scattering (SERS) spectroscopy. Among various recycling strategies, such as thermal treatment, chemical-assisted cleaning, or plasma treatment, photocatalytic degradation represents the most widely used approach for achieving cost-effective and energy-efficient regeneration of SERS substrates. In this context, bifunctional metal–semiconductor nanomaterials are frequently employed to combine high SERS activity provided by plasmonic metallic nanostructures with the photocatalytic ability of metal oxides to degrade molecules adsorbed on the substrate surface.

Here, we investigate niobium pentoxide (Nb_2O_5) with Au and Ag coatings as SERS-active platforms recyclable by UV-light irradiation. Nb_2O_5 films were prepared by magnetron sputtering deposition of approximately 100 nm thick Nb layer onto polished Si wafers, followed by thermal annealing in air to form Nb_2O_5 film. Subsequently, the Nb_2O_5 films were decorated with Au or Ag using planar magnetron sputtering, with deposition times up to 120 s. Using methylene blue (MB) as a model molecule, we demonstrate that the SERS activity of Nb_2O_5/metal coatings is governed exclusively by the plasmonic properties of the metallic nanostructures. At the same time, Nb_2O_5 plays a crucial role in enhancing photocatalytic degradation and cleaning of these hybrid SERS substrates under UV irradiation (253.7 nm). In the case of Nb_2O_5/Au, the complete photodegradation of MB (1×10^{-6} M) is seen after 8 hours. The SERS spectra of a newly deposited MB droplet closely resemble those obtained from a freshly prepared Nb_2O_5/Au substrate, demonstrating the feasibility of repeated reuse (see Figure 1). In contrast, although Nb_2O_5/Ag exhibits more efficient cleaning, the SERS intensity of newly deposited MB reaches only approximately 20% of the original signal before cleaning, indicating partial degradation of the SERS performance.

This work was supported by the grant 25-14402L from the Czech Science Foundation.

Keywords: surface-enhanced, SERS, charge transfer, niobium pentoxide, semiconductor

SERS spectra of MB from niobium pentoxide with Au coating (10 s of Au deposition) before and after UV cleaning.



[Abstract:0198] [Industrial/Societal Applications]

Understanding The Impact of the Fabrication Process On Li-Ion Battery Anodes Using Chemical Analysis with the Strada® Intelligent Raman Microscope

***Jennifer Ferguson*, Andrei Markin, Jorge Diniz, Tim Batten**

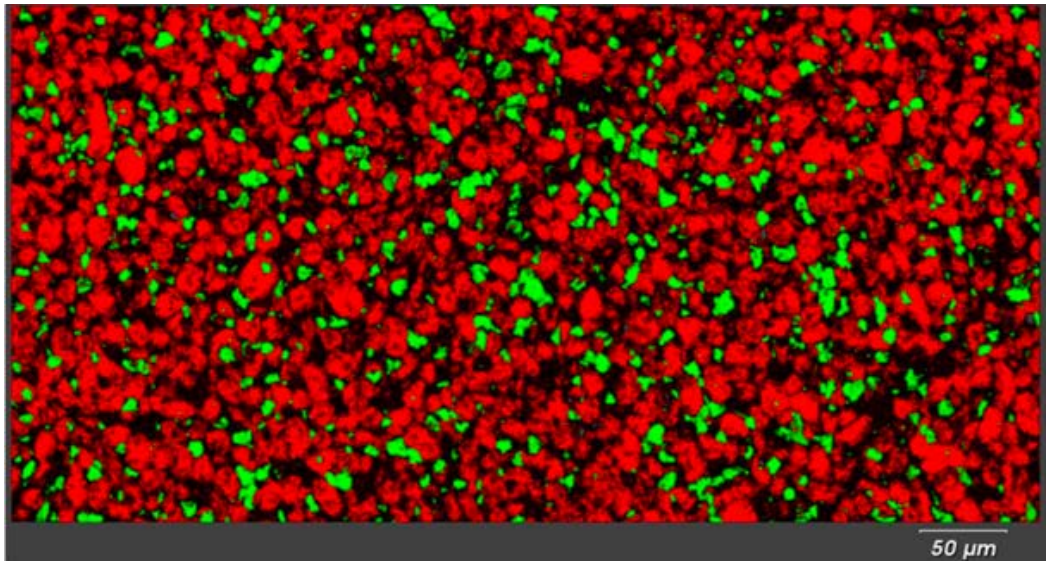
Renishaw PLC, New Mills, Wotton-under-Edge, Gloucestershire, GL12 8JR

Li-ion battery anodes consist of a variety of components and materials, including conductive materials and binders. Different types of carbon are used in anodes to fulfil different purposes, such as participating in intercalation reactions with lithium ions, and providing conducting paths for charge carriers. The performance of Li-ion batteries is strongly influenced by the chemical distribution and particle size of its constituents, which are determined by the fabrication process. Raman spectroscopy is ideally suited as a tool for characterisation of anodes due to its ability to identify different carbon forms and investigate structural and chemical properties of the graphitic and amorphous material.

In this work, the Strada Intelligent Raman microscope was used for the analysis of anodes with changes in the fabrication process. Raman images showing the relative distribution of carbon and SiOx materials allowed for the impact of such changes on the chemical distribution and crystalline properties to be identified (Figure 1). Quantification of the different forms these materials identified relative changes in the amount of amorphous and crystalline content, as well as a reduction in the particle domain sizes, indicating a breakdown of the materials during the mixing process. Variations in the characteristic D and G-bands in the carbon spectrum were analysed to assess the level of disorder and influence of the different preparation methods on the anode structure.

Keywords: Li-ion battery, carbon, anode, SiOx, particle sizing

Figure 1



Raman image showing the chemical distribution of carbon (red) and SiOx (green) across an analysed area on an anode.

[Abstract:0199] [Non-linear/Time-resolved]

Suppressing Spectral Background with Time-Resolved Raman Spectroscopy

***Andrei Markin*, Tim Batten, Jennifer Ferguson, Jorge Diniz**

Renishaw PLC, Wotton-Under-Edge, UK

Fluorescence emission can be orders of magnitude stronger than Raman scattering, which can severely hinder chemical analysis. Time-resolved Raman spectroscopy (TRRS) is a powerful approach to overcome this limitation by exploiting the fast timescale of Raman scattering to separate the Raman signal from other sources of background light.

In this work we show how TRRS can be used to isolate Raman features from unwanted background contributions, including fluorescence induced by the excitation laser and black-body emission from a high-temperature sample. The principles of the technique are described, along with the associated hardware, and resulting measurements from highly fluorescent materials that are difficult to analyse using conventional continuous-wave (CW) Raman spectroscopy.

An example application is shown in Figure 1, where six coloured LEGO bricks (pigment loaded polymers) were measured using both CW Raman spectroscopy and TRRS at 532 nm excitation. The pigments introduce a strong fluorescence baseline and limit penetration depth, making polymer identification challenging in conventional Raman spectra. In each case, TRRS strongly suppresses the fluorescence background and reveals the Raman bands, enabling the polymer to be identified. In the blue and orange bricks, pigment signatures can also be observed, allowing identification as Phthalocyanine Blue and Solvent Orange 3 respectively.

Keywords: Time-resolved Raman spectroscopy, fluorescence suppression, chemical identification

[Abstract:0201] [Novel Approaches]

Sugar Analysis in Honey Using HILIC-Raman Technique

Hirotsugu Hiramatsu

Applied Chemistry, National Yang Ming Chiao Tung University, Hsinchu, Taiwan

The combination of hydrophilic interaction liquid chromatography (HILIC) and Raman spectroscopy is achieved by using a vertical flow (VF) technique that enhances the Raman signal intensity. The VF technique utilizes the total reflection of light in a liquid core waveguide (LCW) of sample solution and improved the efficiency of Raman signal generation and collection. Strong signals of organic solvent, which is required in HILIC, is selectively eliminated by a spatial filter. We report the HILIC-Raman analysis of five sugars (fructose, glucose, sucrose, maltose, and trehalose). The limit of detection (LOD) is 60–80 μg/mL. Also, the HILIC-Raman technique is applied to analyze the sugar content of honey. We demonstrate that the HILIC-Raman technique offers a novel approach of the quantitative analysis of solutes in the LC eluate.

Keywords: hydrophilic liquid chromatography, Raman detection, liquid core waveguide, quantitative sugar analysis

[Abstract:0202] [Materials]

In Situ Confocal Raman Spectroscopy and Microscopy from Cryogenic to Extreme High Temperatures: Monitoring Material Behaviour Across Wide Thermal Ranges

***Miriam Boehmler*[1], *Matthias Finger*[1], *Thomas Meyer*[1], *Wei Liu*[2]**

[1]*Applications, WITec GmbH, Oxford Instruments, Ulm, Germany*
[2]*Applications, Oxford Instruments, Concord, MA, USA*

Confocal Raman spectroscopy and imaging are powerful, non-destructive tools for in situ characterization of materials across a broad thermal range. This contribution highlights the versatility of the technique through three application examples ranging from cryogenic temperatures (<2 K) to 1500 °C, demonstrating its value in both fundamental research and process optimization, complemented by recent advancements in instrument design that further expand its capabilities.

The first case focuses on in situ monitoring of diamond coatings deposited on steel substrates via hot filament chemical vapor deposition (figure 1a+b). A fibre-coupled confocal Raman probe positioned in front of the reactor window enabled continuous acquisition of high-resolution spectra during cooling (870 °C to 30 °C). The resulting data allowed direct quantification of residual thermal stresses within the diamond layer, supporting real-time process optimization.

The second example highlights in situ Raman spectroscopy and imaging in high-temperature chambers up to 1500 °C for the development of refractory materials (figure 1c). Real-time monitoring of phase evolution, chemical stability, and microstructural changes during thermal cycling and sintering provides valuable insights for designing more robust and energy-efficient refractory systems.

A third application (figure 1d) expands the thermal range to low temperatures via cryogenic confocal Raman experiments on two-dimensional materials. Measurements at different temperatures down to 4K (liquid Helium) reveal temperature-dependent phonon behaviour, phase transitions, and strain effects. These results demonstrate the sensitivity of Raman spectroscopy for probing quantum and lattice phenomena in low-dimensional systems.

Together, these studies showcase how confocal Raman spectroscopy enables spatially resolved, real-time analysis of material behaviour from cryogenic to extreme high temperature conditions, thereby accelerating advances in materials research and engineering.

Keywords: Ceramics, Coatings, 2D Materials, High-temperature, Cryogenics

Raman spectroscopy and imaging at extreme temperatures

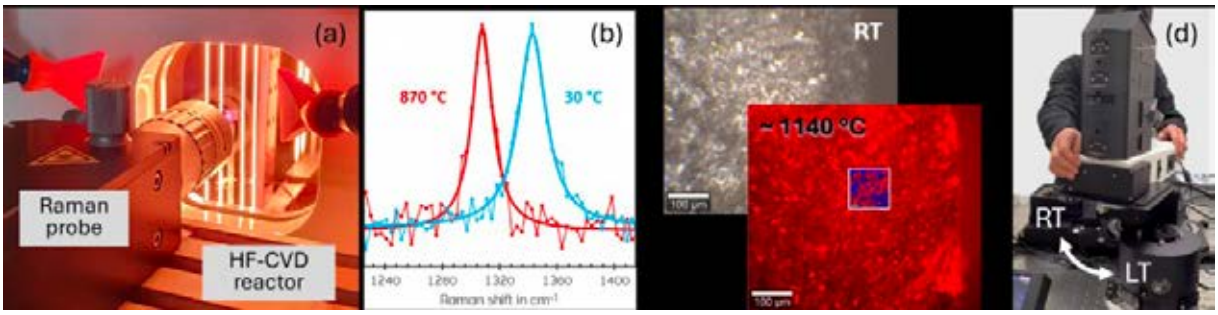


Figure1. a) Mobile confocal Raman probe positioned in front of a CVD chamber. b) Raman spectra of diamond coating measured at 870 °C (red) and 30 °C (blue) during cooling in the chamber. c) Brightfield images measured in a heating stage ranging up to 1500 °C, with a Raman image inset measured at around 1140 °C. d) Confocal Raman imaging system on an optical table with integrated cooling stage for measurements at temperatures as low as 4 K.

Oral Abstracts

[Abstract:0203] [Non-linear/Time-resolved]

Impulsive Stimulated Raman Scattering with Multiple Pump Pulses

***Borui Zhang*[1], *Chrysa Vourdaki*[1], *Luca Genchi*[1], *Randy Bartels*[2], *Liquan Dong*[3], *Hervé Rigneault*[1]**

[1]*Aix Marseille Univ, CNRS, Centrale Med, Institut Fresnel, Marseille, France*
[2]*Morgridge Institute of Science, Madison (WIS), USA*
[3]*School of Optics and Photonics, Beijing Institute of Technology, Beijing, China*

Impulsive Stimulated Raman Scattering (ISRS) employs an ultrashort femtosecond pump pulse to excite molecular vibrations and probe their time-delayed response (1). ISRS is particularly well-suited for investigating low-frequency vibrational modes (<200 cm^{-1}), as these modes are readily excited and probed using standard ~100 fs pulses. In ISRS, a short laser pulse excites all molecular vibrations within its bandwidth (impulsive response). The resulting coherent molecular wave-packet vibration induces a transient refractive index change, which is then probed by a delayed pulse through spectral shift (2) or Kerr lensing (3). However, standard ISRS lacks the ability to selectively excite specific molecular vibrations. In this study, we explore ISRS using multiple pump sub-pulses. By employing an acousto-optic programmable dispersive filter (AOPDF, Dazzler) for the excitation pulse, we generate tailored sequences of sub-pulses to control the molecular wave-packet excitation. We demonstrate that by adjusting the relative timing and amplitude of these sub-pulses, we can selectively enhance or suppress specific vibrational modes, thereby making the recorded spectrum controllable. Our experimental findings are supported by a comprehensive theoretical framework, which shows that N spectral bands can be controlled using a sequence of N+1 sub-pulses. This approach enables spectral manipulation, enhancing the detection of low-concentration species that might otherwise be obscured by strong parasitic spectral lines.

References:

1.R. A. Bartels, D. Oron, and H. Rigneault, "Low frequency coherent Raman spectroscopy," Journal of Physics: Photonics 3, 042004 (2021). https://doi.org/10.1088/2515-7647/ac1cd7

2.S. Metais, S. Suresh, P. Diniz, C. Vourdaki, I. Martin, S. Shivkumar, R. Bartels, N. Forget, and H. Rigneault, "Hyperspectral acquisition with ScanImage at the single pixel level: application to time domain coherent Raman imaging," Optics Express 32, 38849-38863 (2024). https://doi.org/10.1364/OE.533880

3.D. Raanan, J. Lüttig, Y. Silberberg et al., "Vibrational spectroscopy via stimulated Raman induced Kerr lensing," APL Photonics 3, 092501 (2018). https://doi.org/10.1063/1.5029809

Keywords: Impulsive Stimulated Raman Scattering, ISRS, Time domain, multiple pump sub-pulses

[Abstract:0204] [SERS/TERS/Plasmonics]

Enhanced Raman Spectroscopy for Chemical Reactions at Air-Metal Interfaces

David Baschnagel[1], Tim Parker[1], Felix Schneider[1], Bo Zhang[2], Kaixuan Song[2], Jiyong Wang[2], Dai Zhang[1]

[1]Institute of Physical and Theoretical Chemistry, Eberhard Karls University of Tübingen, Germany
[2]Hangzhou Dianzi University, P. R. China

For chemical reactions at the air-metal interface, both activity and selectivity are strongly influenced by factors such as reactant adsorption behavior, the nature of active sites, and interfacial reaction dynamics [1,2,3]. In TERS studies, variations in spectral intensity and the ratios between characteristic peaks are carefully analyzed to identify the occurrence of chemical reactions, elucidate reaction pathways, and evaluate reaction kinetics.

In our recent work, we have demonstrated that TERS signals exhibit angular distribution, with intensities highly sensitive to the orientation of the molecular dipole, the position of the detection element, the tip geometry, the emission wavelength, and other experimental parameters [4,5]. Since spectral intensity serves as a key metric in TERS investigations of chemical reactions, these factors need to be carefully considered to ensure reliable interpretation of experimental results.

In this talk, I will shortly present our ongoing studies of combining back focal plane imaging and energy-momentum spectroscopy with artificial intelligence-assisted Raman data analysis. We explore the capabilities and limitations of enhanced Raman spectroscopy for probing chemical reactions at the air-metal interfaces.

Fundings: This work was supported by the German Research Foundation through funds ZH 279/13-1, ZH 279/15-1, ZH 279/16-1 and by the Sino-German Mobility Program through fund M-0547.

References:

[1] J. J. Sun et al. Role of adsorption orientation in surface plasmon-driven coupling reactions studied by tip-enhanced Raman spectroscopy, Journal of Physical Chemistry Letters, 2019, 10, 2306-2312.

[2] N. Kumar et al. Nanoscale chemical analysis of heterogeneous catalysts using tip-enhanced Raman spectroscopy, Chemical Reviews, 2026, https://doi.org/10.1021/acs.chemrev.5c00707

[3] S. Mennicken et al. Probing a reactive alkyne center aligned via a triphenylmethane tripod on Au(111) for electric field-induced chemistry by STM and TERS, Small, 2026, DOI: 10.1002/smll.202509467

[4] F. Schneider et al. Mini-Review: angular scattering and directional effects in tip-enhanced Raman spectroscopy, Journal of Raman Spectroscopy, 2026; 0:1–20, https://doi.org/10.1002/jrs.70091.

[5] F. Schneider et al. Angularly resolved tip-enhanced Raman spectroscopy, Angew. Chem. Int. Ed. 2025, 64, e202506152, https://doi.org/10.1002/anie.202506152.

Keywords: Enhanced Raman spectroscopy, back focal plane imaging, energy momentum Raman spectroscopy, chemical reaction, AI-assisted data analysis

Oral Abstracts

[Abstract:0206] [SERS/TERS/Plasmonics]

Hyperbolic-Enhanced Raman Spectroscopy of 2D Materials on Natural VdW $MoOCl_2$

***Gleb Tselikov*[1], *Anton Minnekhanov*[1], *Georgy Ermolaev*[1], *Aleksey Arsenin*[1], *Kostya S. Novoselov*[2], *Valentyn Volkov*[1]**

[1]*Emerging Technologies Research Center, XPANCEO, Internet City, Emmay Tower, Dubai, United Arab Emirates*
[2]*Department of Materials Science and Engineering, National University of Singapore, Singapore, 03-09 EA, Singapore*

Natural van der Waals (vdW) crystals with in-plane hyperbolic dispersion represent a new frontier for nanophotonics, offering high-momentum polariton modes and a massive density of optical states without the fabrication challenges of artificial metamaterials [1]. Molybdenum oxychloride (MoOCl2), a quasi-one-dimensional vdW metal, has recently emerged as a unique platform exhibiting broadband hyperbolicity in the visible spectral range [2–5].

In this work, we demonstrate that MoOCl2 serves as a versatile and powerful platform for the study of Raman spectroscopy in atomically thin 2D materials. While MoOCl2 flakes facilitate high-sensitivity surface-enhanced Raman spectroscopy (SERS) for molecular detection [3], its primary advantage lies in its ability to enhance intrinsic signals from other vdW layers. We show that placing graphene, hexagonal boron nitride (hBN), or MXenes on MoOCl2 leads to a dramatic increase in Raman signal intensity - with enhancement factors reaching up to 50 times compared to standard dielectric substrates [3].

A defining feature of this "Hyperbolic-Enhanced Raman" (HypER) scattering is its extreme anisotropy. We observe that the Raman enhancement is highly sensitive to the polarization of the excitation laser relative to the MoOCl2 crystal axes. Specifically, the enhancement factor is approximately 20 times higher when the incident light is polarized along the metallic a-axis compared to the dielectric b-axis [3]. This directional control is a direct consequence of the material's electronic anisotropy and the excitation of low-loss hyperbolic plasmon polaritons (HPPs), which provide a high Purcell factor and deep sub-wavelength light confinement [5].

Our findings establish MoOCl2 as a lithography-free, wafer-compatible platform for the advanced spectroscopic characterization of 2D materials across the visible and telecommunication bands [2-3]. By leveraging natural hyperbolicity, we provide a new paradigm for enhancing light-matter interactions in vdW heterostructures, offering a superior alternative to traditional metamaterial-based sensing [6].

References:

1. Gjerding, M. N. et al. Nat. Commun. 8, 320 (2017).

2. Ermolaev, G. et al. arXiv:2512.06495v1 (2025).

3. Minnekhanov, A. et al. arXiv:2512.17647v1 (2025).

4. Li, Y. et al. Nat. Commun. 16, 6172 (2025).

5. Ruta, F. L. et al. Science, 387(6735), 786–791 (2025).

6. Li, D. et al. Microsyst. Nanoeng. 11, 60 (2025).

Keywords: van der Waals materials, MoOCl2, hyperbolic materials, Raman spectroscopy, SERS

Oral Abstracts

[Abstract:0207] [SERS/TERS/Plasmonics]

Angular Distribution of Tip-Enhanced Raman Scattering

***Felix Schneider*[1], *Tim Parker*[1], *Liangxuan Wang*[1], *Michel Rebmann*[1], *Yang Zhao*[1], *Eric Juriatti*[1], *Heiko Peisert*[1], *Alfred J. Meixner*[1], *Johannes Gierschner*[2], *Lingyan Meng*[3], *Dai Zhang*[1]**

[1]*Institute for Physical and Theoretical Chemistry, University of Tübingen, Germany*
[2]*Madrid Institute for Advanced Studies, IMDEA, Universitaria de Cantoblanco, Spain*
[3]*School of Physics and Physical Engineering, Qufu Normal University, P. R. China*

Tip-enhanced Raman scattering (TERS) is a powerful technique that enables the investigation of the optical response of individual molecules with spatial resolution beyond the optical diffraction limit. Recent developments have allowed the visualisation of sub-molecular features on the Ångström scale through variations in Raman spectra. To achieve this, several experimental geometries have been developed, including top-, bottom-, and side-illumination configurations. Each configuration inherently introduces a collection bias determined by parameters such as the numerical aperture, collection angle, and optical pathway. Theoretical studies indicate that the specific geometry of the probing tip can significantly affect the far-field emission pattern of the TERS signal. Consequently, the signal-collection geometry becomes an important factor for comparing quantitative spectral features obtained with different tips or microscopes. This aspect is rarely addressed in experimental studies.

We report the first experimental study of angle-resolved far-field emission in TERS. We reveal peak-dependent emission directionality of TERS signal [3]. The experiment is performed by resonantly exciting a gap-plasmon formed between a gold tip and a flat gold substrate to enhance the Raman scattering of a cobalt-hexadecafluorophthalocyanine (CoPcF16) bilayer. The scattered light is collected in a top-illumination configuration using a parabolic mirror with a high numerical aperture of NA ≈ 0.9986 in air. This setup enables detection over the entire azimuthal range of $\varphi = 0°$ to 360° and a large polar range $\theta = 27°$ to 87° relative to the optical axis. Spatial filtering in the back-focal plane is employed to isolate signals originating from selected solid-angle regions, which allows direct comparison of the corresponding TERS spectra. Supported by (TD)DFT and FDTD calculations, the observed emission directionality of the Raman bands in gap-mode configuration can be attributed to two main effects: (1) The geometry of the vibrational modes responsible for the Raman response, and a reduction of the molecular symmetry from D4h to C4v, which activates Raman bands that were inactive in free space. (2) Resonance matching between the Raman scattering and the gap-plasmon, which influences the enhancement strength and the emission directivity of the system.

Keywords: TERS, back-focal plane, energy-momentum spectroscopy, directionality, angle-resolved

[Abstract:0210] [Coherent Raman Imaging]

Hybrid CW–Pulsed Coherent Anti-Stokes Raman Scattering

***Ruidong Ji*[1], *John F. Kerr*[1], *Tim Batten*[2], *Daniel Wolverson*[1], *Ventsislav K. Valev*[1]**

[1]*Department of Physics, University of Bath, Bath, BA2 7AY, UK.*
[2]*Renishaw plc, New Mills, Kingswood, GL12 8JR, UK.*

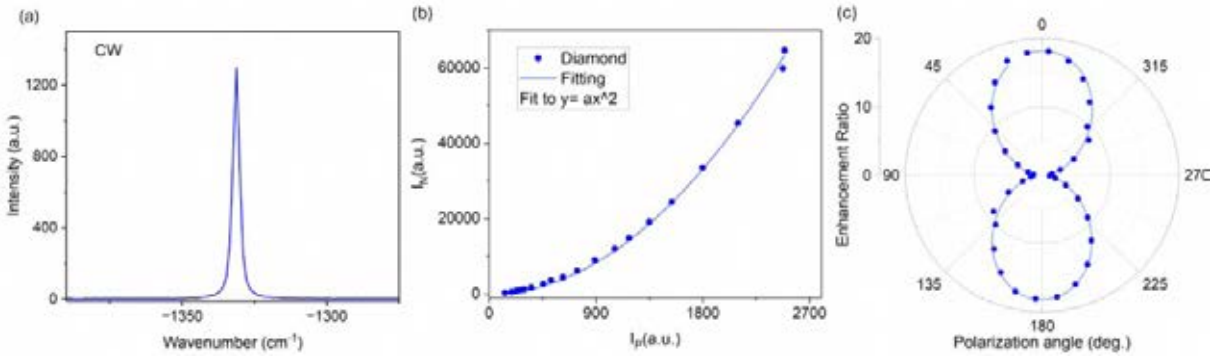
We demonstrate a microscopy scheme for hybrid coherent anti-Stokes Raman scattering (CARS) using a continuous-wave (CW) pump laser and a tunable pulsed Stokes laser for vibrational imaging and defect characterization in crystalline materials. CARS microscopy is a nonlinear spectroscopic technique that enables label-free imaging based on vibrational contrast. Because the signal scales quadratically with pump intensity and linearly with Stokes intensity, it can provide stronger signals than spontaneous anti-Stokes Raman scattering, making it attractive for high-resolution spectroscopic imaging of complex materials. Crystalline materials with large bandgaps are widely used in demanding environments such as aerospace optics, high-power laser systems, and radiation-resistant windows. However, lattice defects can degrade optical performance, making non-destructive characterization methods increasingly important.

Despite its advantages, the implementation of CARS microscopy typically requires sophisticated laser systems. Conventional CARS microscopy typically requires two synchronized pulsed lasers to achieve sufficiently high peak intensities. While such systems provide excellent performance, they involve complex synchronization and high cost. In contrast, configurations based on two CW lasers offer improved stability and simpler instrumentation but usually suffer from limited enhancement and tunability.

In this work, we present a hybrid excitation approach combining a CW pump laser with a tunable pulsed Stokes laser to generate nonlinear anti-Stokes signals. This configuration maintains strong nonlinear excitation during the pulsed interaction while avoiding the need for fully synchronized pulsed laser systems. Figure 1(a) shows the anti-Stokes spectrum of a polycrystalline CVD diamond window under CW excitation. Figure 1(b) presents the dependence of the measured signal on pump excitation and on combined pump + Stokes excitation of the diamond. The data follow a quadratic trend with pump power, consistent with the expected scaling of third-order nonlinear processes. Figure 1(c) shows the variation of the enhancement ratio as a function of the relative polarization between the pump and Stokes beams. Microscopic mapping obtained using both spontaneous Raman scattering and the nonlinear signal will also be presented, highlighting differences in imaging contrast and signal enhancement between the two approaches

Keywords: Coherent anti-Stokes Raman scattering, Microscopy, Nonlinear optics

Figure 1



Nonlinear anti-Stokes signal measured from a polycrystalline CVD diamond window using a CW pump and pulsed Stokes excitation. (a) Anti-Stokes spectrum under the CW excitation. (b) Nonlinear intensity as a function of pump intensity. The solid line shows a quadratic fit to the data. (c) Enhancement ratio as a function of the relative polarization angle between the pump and Stokes beams.

[Abstract:0211] [SERS/TERS/Plasmonics]

Quantitative SERS of PEDOT:PSS Using Nanocellulose–Au@Ag Nanowire Composite Films

***Ario Jafari*[1], *Yuyang Li*[2], *Klas Tybrandt*[2], *Thomas Ederth*[1]**

[1]*Division of Biophysics and Bioengineering, Department of Physics, Chemistry and Biology, Linköping University, SE-58183 Linköping, Sweden*
[2]*Laboratory of Organic Electronics, Department of Science and Technology, Linköping University, SE-60174 Norrköping, Sweden.*

PEDOT:PSS is a conducting polymer for biointerfaces, soft sensors, and organic electrochemical devices, where performance depends sensitively on microstructure and doping. In routine workflows, these material states are often inferred indirectly (e.g., from electrical tests), while Raman spectroscopy could provide a direct chemical and structural explanation but is frequently too weak for thin films and interfacial layers. A practical surface enhanced Ranan spectroscopy (SERS) approach must therefore do two things at once: enhance signal and remain reproducible despite the tendency of plasmonic nanostructures to aggregate. Here we use a cellulose nanofibril (CNF) scaffold to stabilize plasmonic Au@Ag nanowires, forming flexible, water-processable composite films with accessible and repeatable hotspots. We first compare normal Raman of 1 g/L PEDOT:PSS on glass with SERS spectra obtained from several AuNR-based formats (Fig. 1a). The PEDOT Cα=Cβ symmetric stretch serves as a robust single-band metric for substrate benchmarking, and the CNF-containing composites deliver the strongest response. We then move from benchmarking to quantification by recording a concentration series on an AuNR:CNF (2:1) composite from 1 g/L down to 100 ng/L (Fig. 1b). The peak intensity follows a log–log linear calibration across the tested range, enabling concentration estimation and yielding a PEDOT detection limit of 18–40 ng/L under these conditions. Importantly, the spectra still report on polymer state, the main PEDOT band shifts and sharpens relative to normal Raman while PSS-related features are suppressed, consistent with adsorption-associated structural and doping changes near plasmonic sites. Together, these results show that CNF-stabilized Au@Ag nanowire composites can turn SERS into a quantitative and information-rich probe of PEDOT:PSS, supporting process optimization and quality control for polymer electronics and biointerfaces.

Figure 1. (a) Raman spectrum of 1 g/L PEDOT:PSS on glass substrate and SERS spectra of different SERS samples. (b) Raman spectrum of 1 g/L PEDOT:PSS on glass substrate and Raman spectra of different concentrations of PEDOT:PSS on an AuNR:CNF (2:1) composite SERS substrate (λ_0 = 532 nm, 10 mW, 30 s).

Keywords: SERS, PEDOT:PSS, nanocellulose, Au@Ag nanowires, polymer electronics

Figure 1

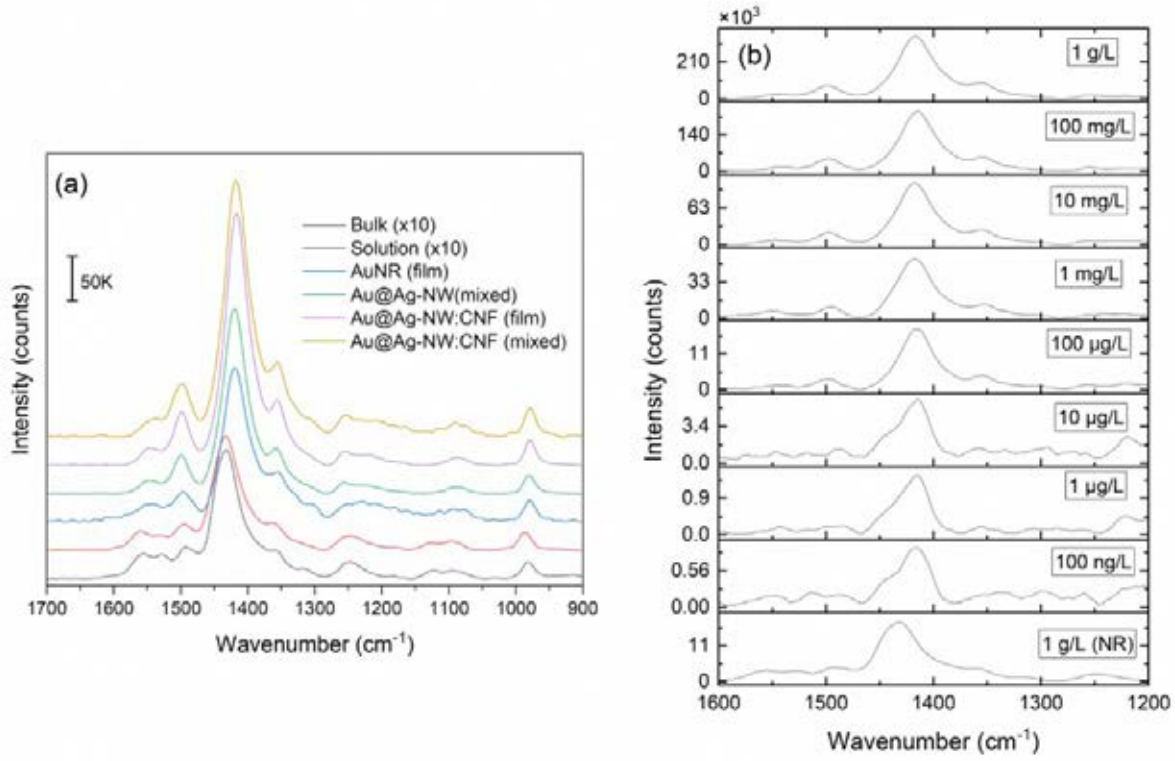


Figure 1. (a) Raman spectrum of 1 g/L PEDOT:PSS on glass substrate and SERS spectra of different SERS samples. (b) Raman spectrum of 1 g/L PEDOT:PSS on glass substrate and Raman spectra of different concentrations of PEDOT:PSS on an AuNR:CNF (2:1) composite SERS substrate (λ_0 = 532 nm, 10 mW, 30 s).

[Abstract:0215] [Industrial/Societal Applications]

Pigment Diversity and Unusual Blue Biogenic Shell in the Invasive Population of Rapana Venosa Sea Snail Revealed by Multi-Laser Raman, SERS, FT-IR, XRD, and SEM-EDX Analysis

***Iuliana-Cornelia Sandu-Poplăcean*[1], Dănuț-Alexandru Dumitru[2], Fran Nekvapil[3], Geza Lazăr[1], Karlo Maškarić[3], Tudor Tămaș[4], Lucian Barbu-Tudoran[5], Simona Cîntă Pînzaru[1]**

[1]Ioan Ursu Institute of the Faculty of Physics, Babeș-Bolyai University, 1 Kogălniceanu 400084 Cluj-Napoca, Romania, RDI Institute in Applied Natural Sciences, Babeș-Bolyai University, 30 Fântânele 400327 Cluj-Napoca, Romania.
[2]Ioan Ursu Institute of the Faculty of Physics, Babeș-Bolyai University, 1 Kogălniceanu 400084 Cluj-Napoca, Romania
[3]Ioan Ursu Institute of the Faculty of Physics, Babeș-Bolyai University, 1 Kogălniceanu 400084 Cluj-Napoca, Romania, RDI Institute in Applied Natural Sciences, Babeș-Bolyai University, 30 Fântânele 400327 Cluj-Napoca, Romania, National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donath, 400297 Cluj-Napoca, Romania.
[4]Department of Geology, Babeș-Bolyai University, 1 Kogălniceanu 400084 Cluj-Napoca, Romania.
[5]National Institute for Research and Development of Isotopic and Molecular Technologies, 67-103 Donath, 400297 Cluj-Napoca, Romania, Electron Microscopy Centre, Department of Experimental Biology, Babeș-Bolyai University, Clinicilor 5, 400006 Cluj-Napoca, Romania.

Marine organisms' pigmentation has attracted increasing interest for natural dyes. Molluscan shells are stable biocomposites embedding diverse pigments within a calcium carbonate matrix. However, blue-purple shell coloration remains particularly intriguing and poorly understood. The invasive gastropod Rapana venosa, widely distributed in the Black Sea, exhibits notable chromatic variability, including unusual blue-pigmented shells alongside the more common orange ones. The pigmentary basis of this blue coloration remains unclear.

In this study, we report the first comprehensive spectroscopic characterization of unusual blue and common orange interior-pigmented R. venosa shells using an integrated multi-analytical approach (Figure 1). The study group consisted of 49 specimens collected from the Romanian Black Sea coast, approximately 6 km south of Midia Cape. Shell morphometry showed no correlation with blue coloration. Confocal micro-Raman analysis revealed a pigment gradient across shell layers from aragonite-rich interiors to calcite-dominant exteriors. SEM showed organic fibrils interconnecting mineral crystallites. Resonance and non-resonance Raman analyses employing five laser lines enabled accurate in situ pigment identification, including polyenes, porphyrins, and eumelanin. Multi-laser Raman measurements distinguished at least two classes of polyenes based on the position of the ν_1(C=C) and ν_2(C–C) bands. Blue shells showed ν_1(C=C) below 1500 cm^{-1}, consistent with long-chain methylated polyenes, whereas orange shells exhibited ν_1(C=C) above 1500 cm^{-1}, attributed to unsubstituted polyenes. Linear combination and harmonic Raman bands further discriminated the polyene species. Carotenoids were not detectable in situ either with 442 or 532 nm excitation. However, ethanol extraction followed by SERS analysis with AgNPs revealed β-carotene as the only extractable pigment. FT-IR spectra showed broad mineral bands and traces of organic components associated with aliphatic $-CH_2$/ $-CH_3$ groups, while powder X-ray diffraction confirmed dual polymorphism. SEM-EDX analysis excluded structural coloration and revealed micrometre-scale crystal layer organization with trace heavy metals.

Overall, the results provide first comprehensive pigment characterization in Rapana venosa intact biomatrix and highlight the powerful Raman technology combined with ultrafast, ultrasensitive detection capability for complex analyses. The unusual blue coloration of certain R. venosa shells arises from a complex pigment interplay involving polyenes, eumelanin, and porphyrins embedded within the shell matrix, while purple indigotin and blue carotenoproteins were excluded.

Keywords: β-carotene, Eumelanin, Long-chain polyenes, Resonance Raman, Unusual blue gastropod shell.

Figure 1. The analytical workflow and main spectroscopic findings of the study.

[Abstract:0219] [SERS/TERS/Plasmonics]

Probing Intracellular Interactions of Functionalized Nanoparticles for Organelle Targeting with SERS

Cecilia Spedalieri, Janina Kneipp

Department of Chemistry, Humboldt-Universität zu Berlin, Berlin, Germany

The use of nanostructures for biomedical and theranostic applications relies on their successful uptake by the targeted cells and delivery to different organelles. Unless they are specifically targeted to a particular organelle, all particles will transit through the endolysosomal pathway of an animal or human cell. Targeting can be achieved, amongst other methods, by using molecules with known affinity for certain cellular structures or via functionalization with specific peptides that act as localization signals and indicate the delivery destination, with a specific sequence for each organelle. However, functionalization does not guarantee that the probe will reach its intended destination.[1] To improve the success of targeted delivery, it is important to understand the effect of functionalization on cellular processing of nanoparticles and how the nanoparticle-biomolecule interactions affect the delivery of the cargo. In particular, surface-enhanced Raman scattering (SERS) spectroscopy is a sensitive tool to monitor intracellular interactions of plasmonic nanoparticles.[2,3] Mitochondria are vital organelles in cells, and their dysfunction contributes to the development of many diseases, including cancer, making the success of targeted theranostics critical.

In this work, we used gold nanoparticles functionalized with mitochondria targeting molecules and studied their interactions with the intracellular biomolecular environment by SERS probing. To functionalize the nanoparticles we used two different molecules: (6-aminohexyl)triphenylphosphonium bromide (TPP), a lipophilic cation widely used for molecular delivery to mitochondria and elamipretide, a short peptide that binds selectively to cardiolipin in the inner mitochondrial membrane. Depending on the surface modification, and how the molecules are bonded to the nanoparticles, the SERS signals show differences in the interactions with different biomolecules such as proteins and lipids. Functionalized gold nanoparticle distribution and aggregation in the cells and the cellular ultrastructure were imaged by soft X-ray tomography, showing that interparticle interactions are affected by the surface functionalization. Understanding how these molecules affect nanoparticle interactions with cellular environments will help improve targeted delivery.

References:

[1] Drescher D, Büchner T, Schrade P, Traub H, Werner S, Guttmann P, Bachmann S, Kneipp J, ACS Nano 2021, 15

[2] Kneipp J, Seifert S, Gaerber F, Chem Soc Rev 2024, 53

[3] Spedalieri C, Kneipp J, Nanoscale 2022, 14

Keywords: Nanoparticles, SERS, particle functionalization, targeting molecule, mitochondria

[Abstract:0220] [SERS/TERS/Plasmonics]

Dual-Enhanced SERS Platforms Using Edge-Engineered Graphene Quantum Dots and Silver Nanoshells

Hyejin Chang

Division of Science Education, Kangwon National University, Chuncheon, Republic of Korea

Surface-enhanced Raman scattering (SERS) enables highly sensitive molecular detection through the plasmonic amplification of local electromagnetic fields. In this work, we present hybrid plasmonic–graphene nanostructures designed to achieve dual-mode SERS enhancement by combining electromagnetic and chemical amplification mechanisms.

Our approach builds on silica-based silver nanoshell architectures that generate strong localized electromagnetic fields. Edge-engineered graphene quantum dots (GQDs) are introduced as additional signal-amplifying components that promote analyte adsorption and facilitate charge-transfer interactions at the metal–graphene interface.

The resulting graphene–plasmonic hybrid nanostructures exhibit synergistic enhancement arising from the coupling between plasmonic hot spots and chemically active graphene edges. By tuning the structural configuration of the nanoshell–GQD assemblies, we demonstrate controllable modulation of Raman signal intensity and analyte affinity, leading to improved sensitivity and selectivity.

These findings provide insight into the cooperative roles of plasmonic nanostructures and graphene-based materials in SERS and offer a modular strategy for designing advanced spectroscopic sensing platforms.

Keywords: Surface-enhanced Raman scattering (SERS), Graphene quantum dots, Plasmonic nanoshells; Dual-mode enhancement

[Abstract:0226] [Novel Approaches]

Overcoming Precision Limits in Raman Spectroscopy: A Validated Strategy for Fast and Accurate Dual Axis Calibration

***Konstantinos Stergiou*[1], *Yaroslav Aulin*[2], *Yurii Pilhun*[2], *Danylo Komisar*[2], *Andrii Kutsyk*[2], *Martin A.B. Hedegaard*[3], *Oleksii Ilchenko*[2]**

[1]*Lightnovo ApS, Blokken 11, 1., Birkerød, 3460, Denmark, Department of Green Technology, University of Southern Denmark, Odense M, Denmark*
[2]*Lightnovo ApS, Blokken 11, 1., Birkerød, 3460, Denmark,*
[3]*Department of Green Technology, University of Southern Denmark, Odense M, Denmark*

Calibration accuracy and reproducibility are critical for repeatable classification models and quantitative analysis in Raman spectroscopy. Although modern Raman instruments now offer performance specifications capable of addressing challenging applications such as bacterial identification, blood glucose quantification, and fermentation process monitoring, the transferability of calibration models between devices remains limited due to fundamental uncertainties in calibration accuracy. As a result, impressive proof-of-concept results cannot easily be translated into widely deployable industrial solutions.

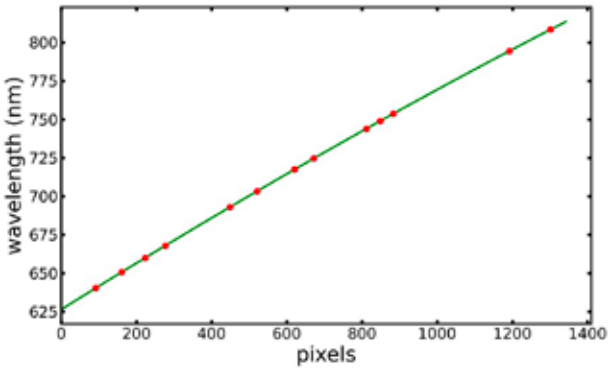
Wavenumber calibration based on Raman-active materials is typically limited in accuracy due to potential mismatches among spectral libraries and Raman standards, as well as the inherent uncertainty in determining the positions of composite and asymmetric peaks. Similarly, calibration using atomic emission lines is prone to errors due to differences between the optical path of the emission source and that of the Raman signal. Moreover, uncertainty in the laser wavelength further increases the overall error. Finally, intensity correction methods typically neglect the instrument's polarization response resulting in additional uncertainty into the measured signal.

In this work, we introduce a novel dual-axis calibration procedure that addresses these uncertainty sources and we provide a validated spectral library for Raman samples referenced in ASTM standards. For that reason, we developed a polarized Raman spectrometer based on a Wollaston prism analyzer. Our calibration approach cancels the aforementioned optical path mismatch, enabling reliable calibration using emission sources with well-defined peak centroids (Figures 1 and 2). The calibration accuracy is further validated against independent atomic emission lines, such as Krypton, showing a calibration error below 0.04nm (Figure 3). Accurate transformation to Raman wavenumber is ensured by continuously monitoring the excitation laser wavelength through a reference channel (Figure 4). Additionally we constantly correct the intensity accounting for the polarization-dependent instrument response (Figures 4, 5 and 6).

The proposed framework is validated across five different instruments through cross-platform measurements and transferability tests on classification models developed for bacteria identification after cultivation.

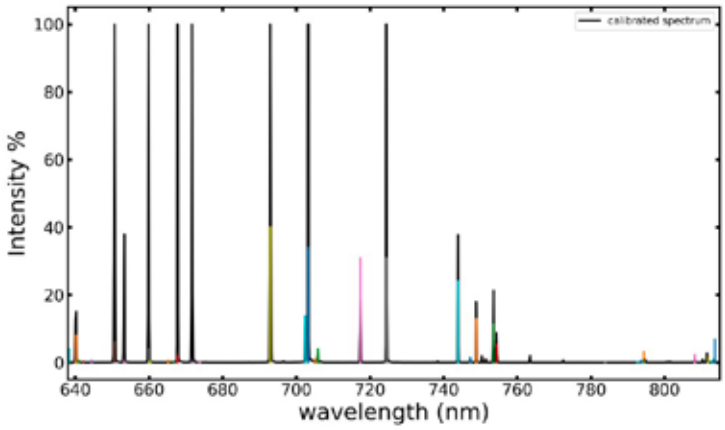
Keywords: Calibration, Calibration transfer, Calibration models

Figure 1. Wavelength Calibration Polynomial.



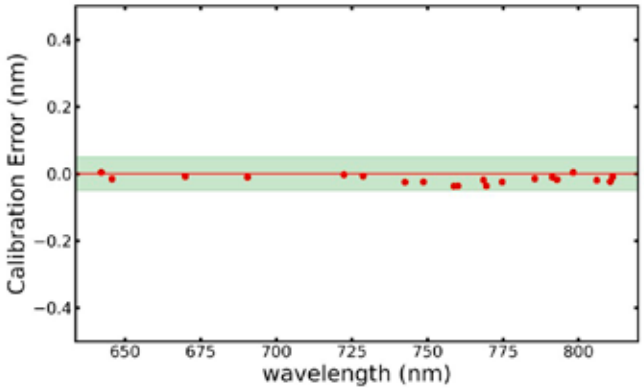
Wavelength calibration of the 638 nm Raman spectrometer using a fourth-order Chebyshev polynomial. Red points indicate the measured neon emission lines used as calibration references, and the green curve represents the resulting best-fit polynomial.

Figure 2. Comparison of Calibrated Neon Emission Spectrum with NIST Reference



Calibrated neon emission spectrum acquired with the 638 nm Raman spectrometer overlaid with the reference spectrum from the National Institute of Standards and Technology (NIST). The alignment of spectral peaks demonstrates the accuracy of the wavelength calibration

Figure 3. Calibration Error of Krypton Spectrum Relative to NIST Reference



Calibration error of the measured krypton spectrum relative to the NIST reference, demonstrating an error < 0.04 nm (< 1cm-1 for 638nm laser source).

Figure 4. Raman Detection Channels

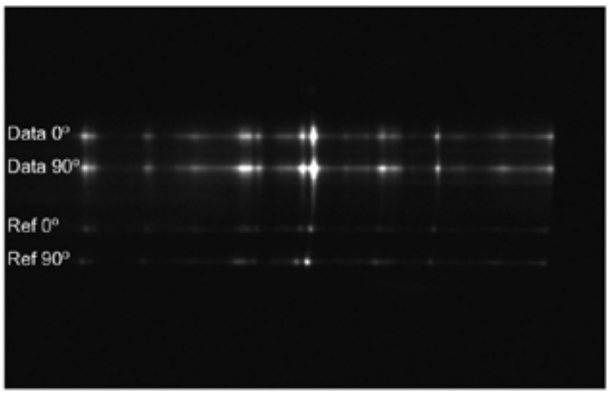
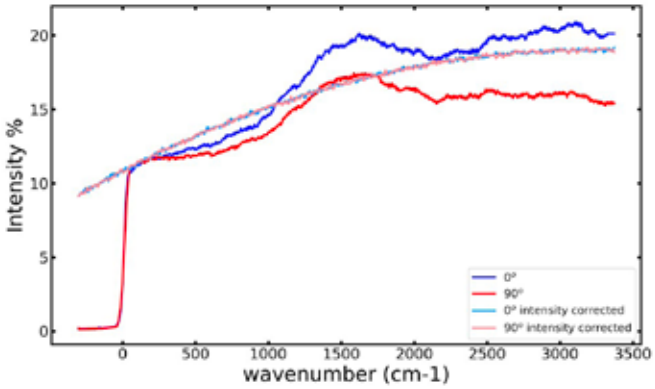


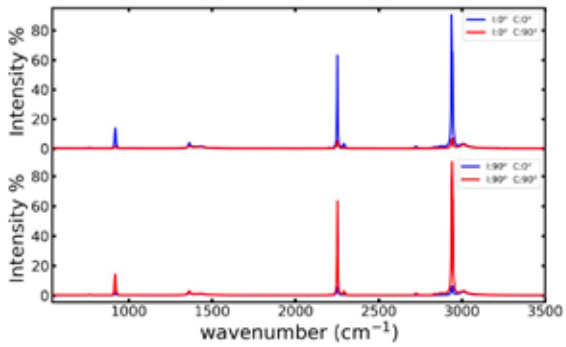
Image of the sensor illustrating the spectral and reference channels corresponding to the two orthogonally polarized Raman detection paths. This configuration enables real-time monitoring of laser wavelength variations while simultaneously supporting corrected polarization-resolved Raman measurements.

Figure 5. Polarization-Dependent Instrument Response Correction



Correction of the polarization-dependent instrument response. Intensity calibration is performed separately for each polarization detection channel to ensure accurate relative Raman signal comparison.

Figure 6. Intensity-Corrected Polarization-Resolved Raman Spectra of Acetonitrile



IIntensity-corrected Raman spectra of acetonitrile measured under 0° and 90° incident polarization states and simultaneously detected in the corresponding polarization channels. Blue lines correspond to the 0° polarization detection channel and red lines to the 90° channel. The upper panel shows spectra acquired with 0° incident polarization, while the lower panel shows spectra acquired with 90° incident polarization. The agreement in peak intensities and ratios for equivalent polarization configurations demonstrates the effectiveness of the polarization intensity correction.

[Abstract:0227] [Coherent Raman Imaging]

Metrology for Coherent Raman Scattering Microscopy

***Siddarth Shivkumar*[1], *Dimitrios Tsikritsis*[1], *Vasundhara Tyagi*[1], *Natalie Belsey*[2]**

[1]*Chemical & Biological Sciences Department, National Physical Laboratory, Teddington, UK*
[2]*Chemical & Biological Sciences Department, National Physical Laboratory, Teddington, UK; School of Chemistry & Chemical Engineering, University of Surrey, Guildford, UK*

Coherent Raman scattering (CRS) microscopy offers rapid, high-resolution imaging with Raman contrast. The two main modalities of CRS include coherent anti-Stokes Raman scattering (CARS) and stimulated Raman scattering (SRS) microscopy. Both CARS and SRS are extensively used in biological, biomedical, pharmaceutical, and materials research, with wide-ranging clinical applications. Successful translation and commercialisation of these techniques demand standards to enable harmonised data acquisition and comparison of data acquired on different instruments. Despite the progress, no formal international standards currently exist for CRS microscopy, posing a major obstacle for certified reproducibility and regulatory acceptance.

At present, CRS instruments range from home-built to completely commercial devices and comprise a wide range of hardware (variable laser sources, modulation schemes, detection electronics, as well as optical architectures). The heterogeneity in the hardware inevitably affects the instrument response, which in turn results in a variability in spectral resolution, spatial resolution, sensitivity (signal to noise and signal to background), peak positions, and relative peak intensities. Standards and reference materials with well-known Raman peaks are needed to calibrate the instrument response function. While such knowledge is available for spontaneous Raman spectroscopy, for example, the ASTM E1840 standard proposes a list of reference samples for spontaneous Raman spectroscopy; these samples are not readily suited for CRS microscopy, for which additional optical properties are critical.

The Versailles Project on Advanced Materials and Standards (VAMAS) interlaboratory study aims to take the first step in addressing this issue by testing candidate polymer materials for use as reference standards and measuring the variability in peak position values for CRS microscopy. The samples used in this study cover the spectral ranges of 500 cm-1 to 1800 cm-1 and 2700 cm-1 to 3300 cm-1. Future studies will aim at developing custom samples that cover all spectral ranges, including the lower spectral frequencies (< 500 cm-1) and the spectrally silent region (1800 cm-1 to 2700 cm-1). Establishing such standards will be critical for enabling harmonised data acquisition that is in alignment with regulatory expectations for emerging optical diagnostics.

Keywords: Coherent Raman Scattering Microscopy, Data harmonization, Standardization, VAMAS study.

[Abstract:0230] [SERS/TERS/Plasmonics]

Affinity-Driven SERS Detection of Natural Dyes Using Hydrophobic Interaction and Coordination Bonding

***Sungjun Kwak*[1], *Dae Hong Jeong*[2]**

[1]*Department of Chemistry Education, College of Education, Seoul National University, Seoul, Republic of Korea*
[2]*Department of Chemistry Education, College of Education, Seoul National University, Seoul, Republic of Korea, Learning Science Research Institute, Seoul National University, Seoul, Republic of Korea*

We report a molecular affinity–driven SERS strategy for detecting natural dyes with low metal–surface affinity. Ag bumpy nanoshells provide two surface interfaces: hexadecylamine (HDA)–capped AgNS and mercaptopropionic acid (MPA)–modified AgNS enabling Fe^{3+}-mediated coordination tethering of dyes such as tannic acid and shikonin. The coordination pathway enhances local dye concentration, improving SERS signal-to-noise ratio and lowering detection limits. Mixed-solvent systems further increase dye solubility, enabling sensitive detection of natural dye extracts.

Keywords: Natural dyes, SERS, solvents

[Abstract:0236] [Biology/Biomedicine]

Raman Characterization of Blue Microplastic Ingestion and Carotenoid Responses in Zooplankton

***Ion Nesterovschi*[1], *Matea Marelja*[2], *Inés Segovia Campos*[2], *Karlo Maškarić*[1], *Maria Suciu*[3], *Simona Cîntă Pînzaru*[1], *Bastiaan Ibelings*[2], *Vera Slaveykova*[2]**

[1]*Biomolecular Physics Department, Babeş-Bolyai University, Cluj-Napoca, Romania*
[2]*Department F.-A. Forel for Environmental and Aquatic Sciences, Faculty of Sciences, University of Geneva, Geneva, Switzerland*
[3]*National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania*

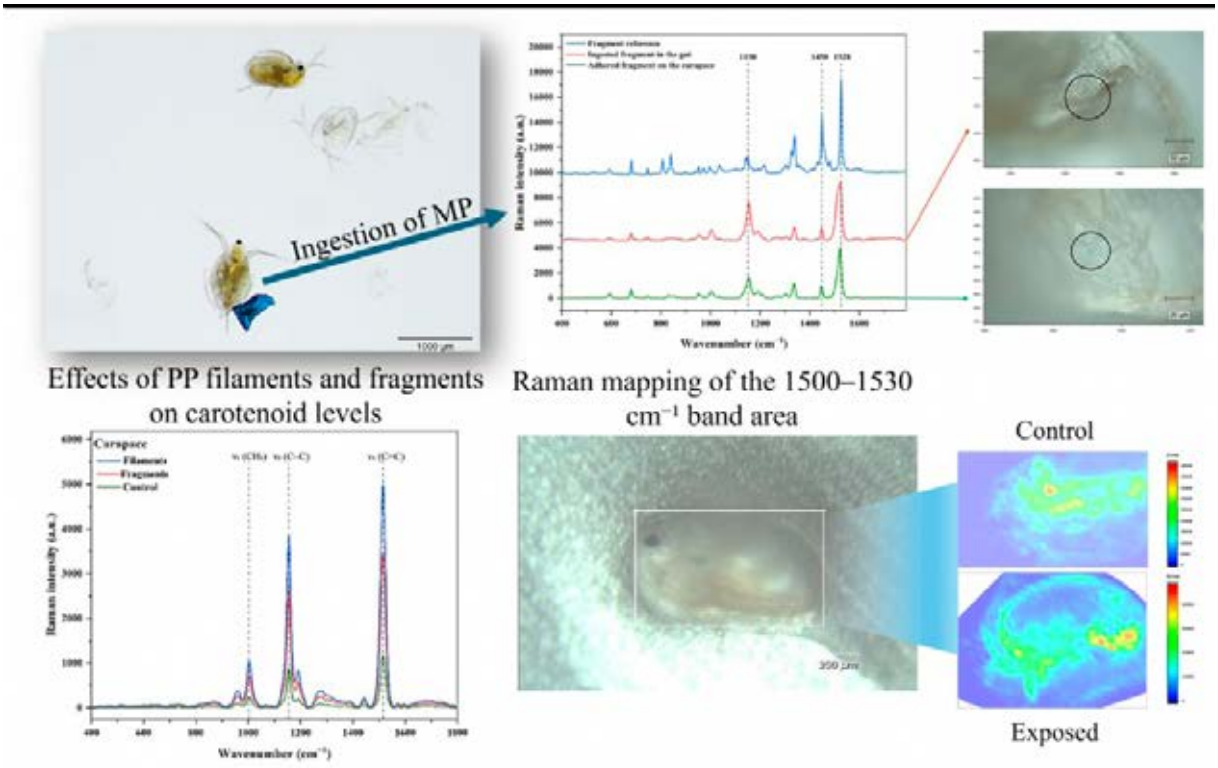
Raman spectroscopy is a very suited technique to describe the microplastic (MP)-organism interactions, enabling polymer identification in the organism, pigment characterisation of the microplastic, and non-invasive evaluation of biochemical stress markers in biological tissue. Here we apply Raman micro-spectroscopy to investigate how two morphologically different forms of naturally aged polypropylene MPs, fibers and fragments, affect two freshwater zooplankton species: Daphnia magna and Thamnocephalus platyurus. The blue PP MPs originated from fishing gear weathered for 15 years in the Adriatic Sea. Raman spectroscopy confirmed their identity as PP (peaks at 1150, 1450, 2880 cm^{-1}) mixed with the copper phthalocyanine pigment PB15 (peaks at 1452 and 1528 cm^{-1}).

After 24h exposure (1000 items per well of fragments and 50 items per well of fibers), Raman micro-spectroscopy with 532 nm laser excitation was used to confirm MP ingestion inside the gut and map carotenoid distribution in the zooplankton as a biochemical stress indicator. PP and PB15 Raman features were detected inside the digestive tract and on the carapace surface of D. magna following fragment exposure, providing direct evidence of ingestion. (Figure 1) Also, the same PP and PB15 bands were detected inside the gut of fiber-exposed D. magna, indicating spontaneous fiber fragmentation during the 24h exposure and ingestion of the resulting particles.

Resonance Raman spectroscopy of the carotenoids present in the zooplankton revealed a consistent, exposure-dependent intensity increase of the three main bands - ν1 (C=C, 1515 cm^{-1}), ν2 (C-C, 1155 cm^{-1}), ν3 (CH3 rock, 1003 cm^{-1}) across gut, heart, carapace, and head body parts of both species. The intensity order filaments > fragments > control, most pronounced in the gut, suggests that carotenoid accumulation represents an antioxidant response to MP-induced stress. Chitin Raman bands dominated the apical spine spectrum of D. magna, confirming the heterogeneous distribution of carotenoids across body tissues. These results demonstrate that Raman spectroscopy is a powerful, label-free tool for simultaneously detecting MP ingestion and monitoring biochemical stress responses in aquatic invertebrates.

Keywords: Raman spectroscopy, microplastics, freshwater zooplankton, carotenoids, ingestion

Figure 1



Raman spectroscopy characterisation of Daphnia magna exposed to naturally aged PP microplastics. (Top) Ingestion of PP fragments confirmed by Raman spectra similar to the reference material, with micrographs showing fragment location. (Bottom left) Carotenoid Raman bands (ν3 = 1003, ν2 = 1155, ν1 = 1515 cm-1) in the carapace, for control, fragment and fiber exposed zooplankton. (Bottom right) Raman intensity map of the 1500-1530 cm-1 band across the whole body of control and exposed animals.

[Abstract:0237] [SERS/TERS/Plasmonics]

Gold Nanoparticle-Catalyzed Oxidation of Beta-Blockers: SERS and Capillary Electrophoresis Study

***Kseniia Makarova*, Elena Solovyeva, Ekaterina Kolobova**

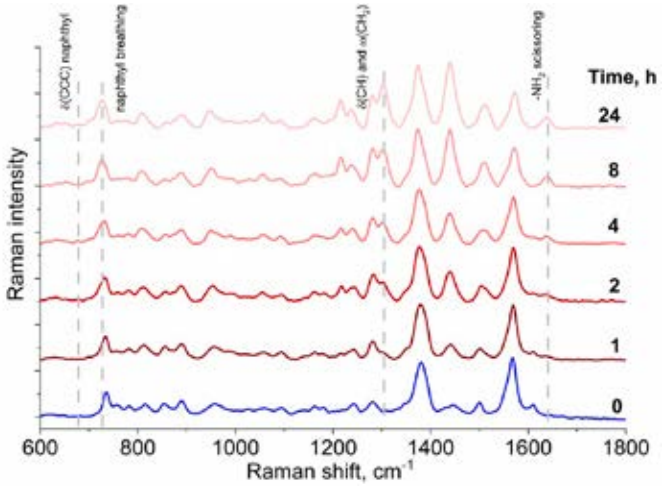
Institute of Chemistry, Saint Petersburg State University, Saint Petersburg, Russia

Gold nanoparticles (GNPs) occupy one of central places in modern nanotechnology due to their abundant properties. Localized surface plasmon resonance (LSPR) underlies the physico-chemical properties of GNPs and causes a number of interface phenomena which do not occur on non-plasmonic surfaces. Precise knowledge and deep understanding of surface processes are crucial to development of bioanalytical applications of gold nanoparticles, for example targeted drug delivery systems, and surface-enhanced Raman scattering (SERS). At the same time, surface transformations, primarily oxidation, involving GNPs have been considered in a number of studies. The complex of these facts makes the study of the interactions of bioactive molecules with GNPs a task of current intense. This work is devoted to the study of interaction of bioactive molecules from a β-blockers family with GNPs. The experiment included the exposure of drug in GNPs dispersion under various conditions, centrifugal separation of GNPs and solution with subsequent analysis of the solid phase by SERS spectroscopy and the liquid phase by capillary electrophoresis (CE). After adsorption of propranolol on the gold surface, a significant change in its SERS spectrum was observed which grew up at increase of incubation time in the nanoparticle dispersion (Fig. 1). Furthermore, an unknown peak appeared in the electropherogram of the liquid phase in addition to two peaks of R and S enantiomers of propranolol. HPLC-MS analysis of the liquid phase showed a presence of N-desisopropylpropranolol. Thus, it was revealed that propranolol is converted into its metabolite on the surface of GNPs by a single-electron transfer mechanism. Subsequent experiments established that reactive oxygen species are formed on the surface of GNPs, and a decrease in their concentration leads to a decrease in the conversion of β-blockers into oxidation products.

The work was supported by Russian Science Foundation, grant № 22-73-10052-P. The authors thank the resource centers of SPBU Research Park: "Chemical Analysis and Material Research", "Optical and Laser Materials Research".

Keywords: gold nanoparticles, SERS, catalysis, beta-blockers

Figure 1. SERS spectra of propranolol after different periods of incubation in GNP dispersion.



[Abstract:0238] [Biology/Biomedicine]

Discrimination and Quantification Of Methotrexate in the Presence of Its Metabolites and Co-Administrated Drugs in Patient Serum Using Lab-On-Disc SERS Platform Supported by Multivariate Data Analysis

***Martyna Anna Pytlarz*, Gohar Soufi, Yaman Göksel, Amalie Løvind Årsten, Roman Slipets, Chen Hsin Liao, Anja Boisen**

Center for Intelligent Drug Delivery and Sensing Using Microcontainers and Nanomechanics (IDUN), Department of Health Technology, Technical University of Denmark, Kongens Lyngby 2800, Denmark.

Surface-Enhanced Raman Scattering(SERS) provides high molecular specificity and sensitivity. However, applying it to complex biofluids such as serum or whole blood remains challenging due to matrix interference. Low reproducibility and the spectral overlap are commonly seen in multi drug treatments. Therefore, the ability to discriminate structurally related compounds, quantify analytes in presence of co-administered drugs and achieve multiplex detection is critical for implementing SERS into clinical use and Therapeutic Drug Monitoring(TDM).

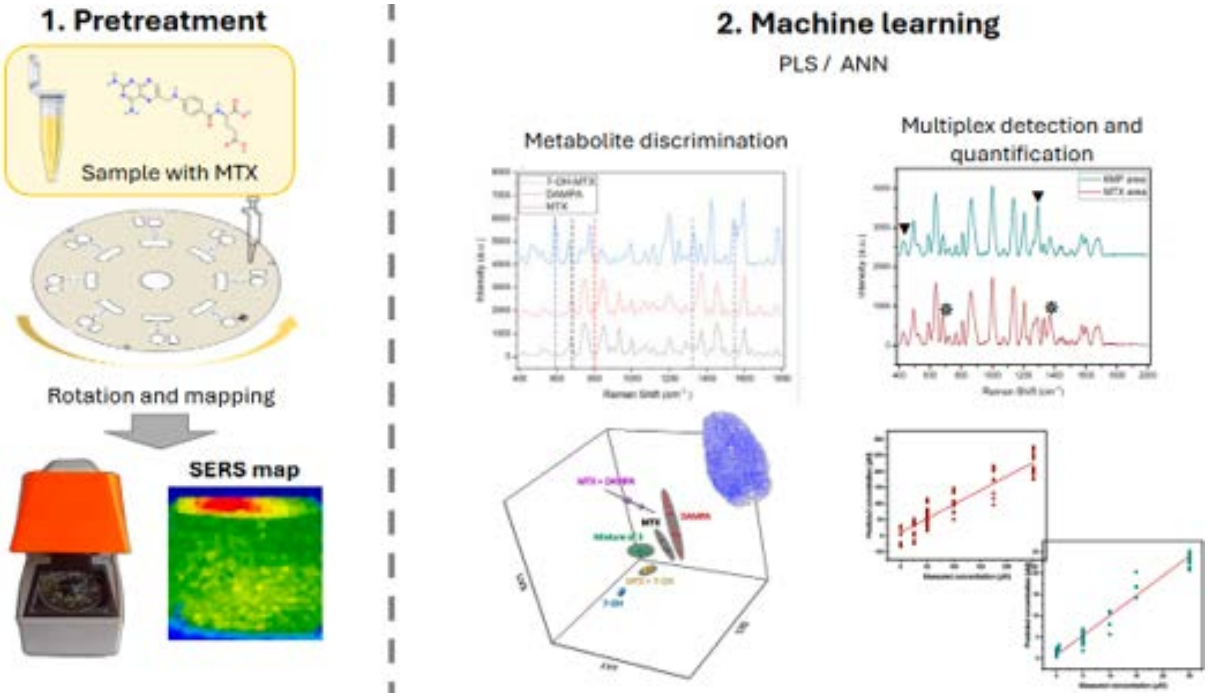
Here, we present integrated lab on disc(LoD) SERS platform that combines filtration and solid phase extraction as sample pretreatment with silver coated nanopillar substrates to enable reproducible, label free detection of small molecule therapeutics in serum. Sample pretreatment performs effective matrix removal while preserving the chemical signature of target analytes, providing a cleaner and consistent input for SERS analysis. The microfluidic disc automates fluid handling through centrifugal forces, for repeatable sample deposition and minimal user intervention.

To address spectral complexity of SERS, we used advanced data analysis tools, including principal component analysis(PCA), partial least squares regression(PLSR), and artificial neural networks(ANNs). In addition to quantification, these approaches were also applied for discriminative analysis, enabling clear classification between drug, its metabolites and co-administrated medication. These chemometric tools helped to extract chemically relevant information and it was demonstrated on methotrexate(MTX), its primary metabolite DAMPA(2,4-diamino-N(10)-methylpteroic acid), and in the mixture containing co-administered drug 6-mercaptopurine (6-MP). Clear differentiation and quantification were shown even when the spectral features partially overlap(Figure 1). Therefore, this approach supports multiplex detection: drugs from different therapeutic classes can be simultaneously analyzed and quantified without the need for labels or assay specific reagents.

The system achieves low micromolar sensitivity across multiple analytes and demonstrates stability in the presence of complex serum backgrounds. Application to MTX patient samples showed good agreement with immunoassay as the reference method, confirming the platform's clinical relevance with recovery of 93%, and recognizing that ICU patients often receive numerous medications that further complicate spectral analysis. By integrating sample pretreatment, automated microfluidics, SERS nanostructures, and multivariate data analysis, this LoD SERS platform provides a scalable, point-of-care solution for multiplex detection and discrimination of drugs in clinically relevant matrices.

Keywords: Surface Enhanced Raman Spectroscopy, Therapeutic Drug Monitoring, Multivariate Data Analysis, Discrimination, Methotrexate

Overall procedure of the drug quantification assay implemented in this work



Oral Abstracts

[Abstract:0241] [SERS/TERS/Plasmonics]

Automated Sample Pretreatment of Complex Matrices on a Centrifugal Microfluidic Platform for Nanopillar-Assisted Separation and SERS Detection

***Gohar Soufi*, Martyna A. Pytlarz, Yaman Göksel, Chen Hsin Tony Liao, Roman Slipets, Anja Boisen**

aCenter for Intelligent Drug Delivery and Sensing Using Microcontainers and Nanomechanics (IDUN), Department of Health Technology, Technical University of Denmark,

Analysis of blood-derived samples remains challenging due to their complex composition and the presence of cells, proteins, and other interfering components that can hinder sensitive molecular detection (Anal. Chem. 2025, 97, 14, 7888–7896). Here, we present a compact analytical system integrating automated sample pretreatment, nanopillar-assisted separation, and surface-enhanced Raman spectroscopy (SERS) for the analysis of drugs in blood and serum samples. The platform incorporates multiple on-chip pretreatment steps designed to efficiently reduce matrix interference prior to detection.

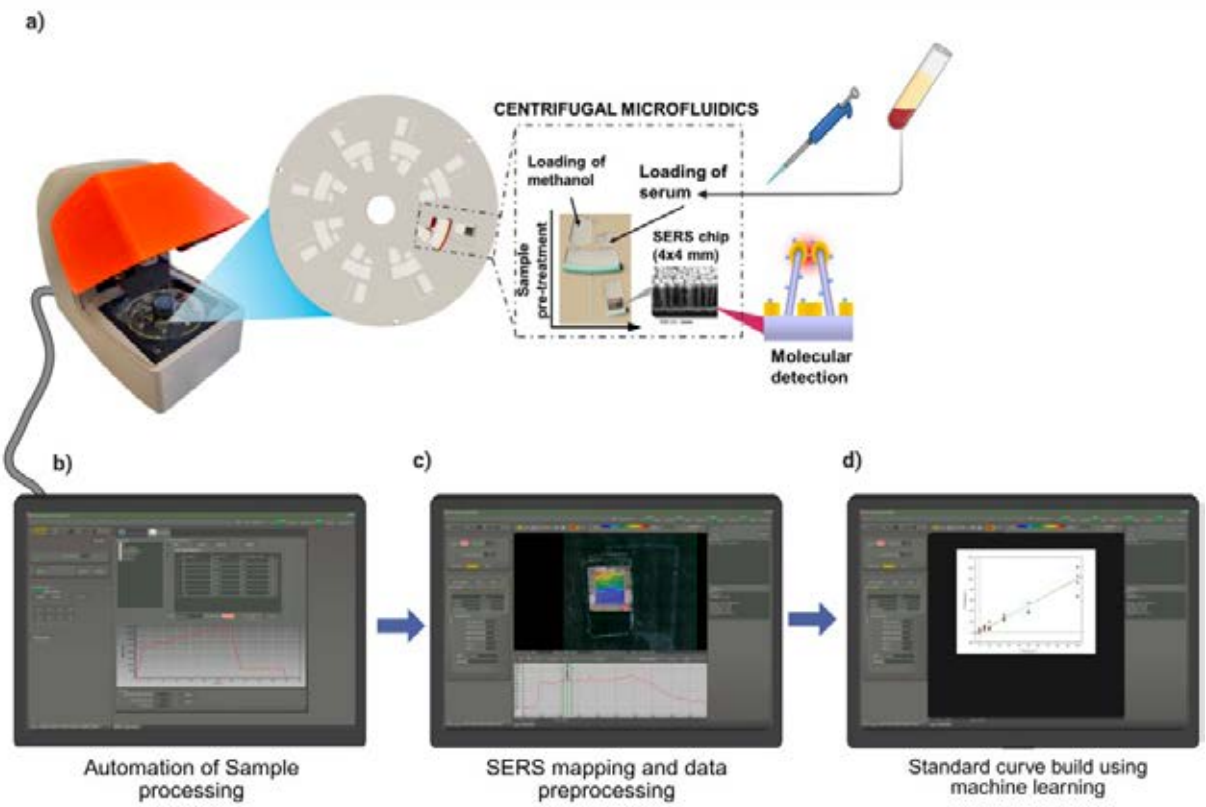
Whole blood samples are first subjected to centrifugal red blood cell separation to isolate plasma from cellular components. The plasma or serum fraction then undergoes controlled dilution and protein precipitation to reduce the influence of high-abundance proteins. Additional purification is achieved through integrated protein precipitation, filtration, or solid-phase extraction (SPE), enabling selective enrichment and cleanup of target analytes from the biological matrix. Following pretreatment, the processed sample is introduced into a nanopillar array that facilitates analyte separation and concentration through size-selective transport, enhanced surface interactions, and increased surface area provided by the nanostructured architecture.

The enriched analytes are subsequently detected using SERS, allowing rapid and label-free molecular identification based on characteristic Raman fingerprints. The integration of automated multistep sample preparation with nanopillar-assisted separation and SERS detection within a compact system reduces manual handling, improves reproducibility, and enhances detection sensitivity.

This approach provides a promising strategy for rapid and reliable analysis of complex biofluids and highlights the potential of combining advanced microfluidic sample preparation with nanostructured separation and spectroscopic detection for clinical and point-of-care applications.

Keywords: Lab-on-disc, Sample pre-treatment, SERS detection

Figure1



Complete analytical process for drug quantification from serum/blood samples (a) photo of the D-SERS system and image of the simplest design of disc, where schematically is shown the processes happening during sample processing (b) screenshot of the software operating the automated spinning of the disc for sample processing, enabling the mixing and step-by-step migration of sample on the SERS chip placed in the sensing chamber by D-SERS (c) software facilitating SERS chip mapping, preprocessing; and (d) advanced data analysis using with machine learning algorithms for drug quantification.

[Abstract:0242] [SERS/TERS/Plasmonics]

Conducting Polymer-Functionalized Gold Nanoparticles as a Reactive Oxygen Species SERS Reporters

***Barbara Palys*, Kacper Jędrzejewski, Hanna Kaflik, Krystian Pupel**

Faculty of Chemistry, University of Warsaw, Poland

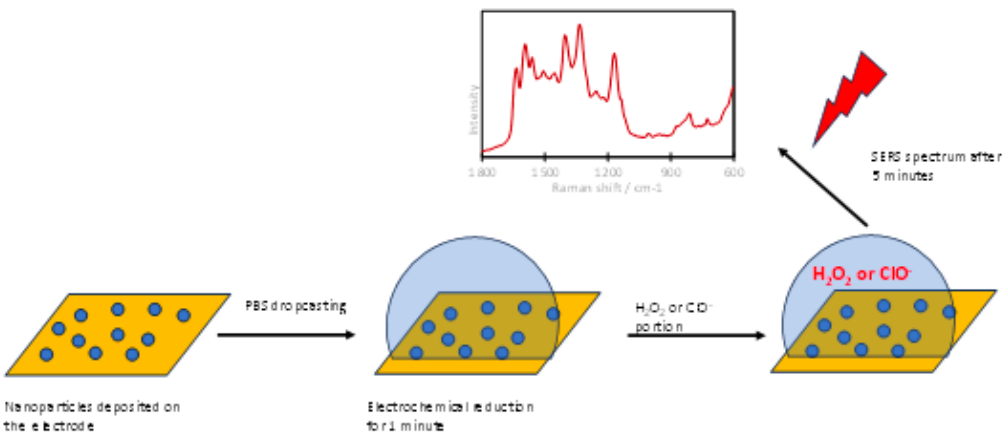
Reactive oxygen species (ROS) are important factors of numerous biological processes. They regulate cell survival, differentiation, inflammation, and defense. Their concentration is regulated by enzymes and antioxidant molecules in healthy tissues. If such mechanism fails, the oxidative stress occurs, which is harmful for DNA and proteins. The concentration of ROS is also important for industrial processes.

Conducting polymers show strong Raman spectra, which depend on the redox potential of their environment in the very wide potential range. These properties make them promising candidates for Raman reporters of the redox state. In this work we study gold nanoparticles wrapped in the thin layer of polyaniline (PANI@AuNPs) or in the layer of poly-3,4-ethylenedioxythiophene (PEDOT@AuNPs). We study their Surface Enhanced Raman Spectroscopy (SERS) spectra upon applied potential in the electrochemical cell. Such experiments are used to calibrate their response to a redox potential. The nanoparticles are characterized using cyclic voltammetry, electrochemical impedance, UV-Vis, DLS, SEM and TEM techniques. Results show, that thin layer of polymer surrounding the nanoparticle may have different properties than bulk polymer, for example PANI@AuNPs are electroactive in a wide pH range (3-8) unlike PANI films active in acidic solutions, what is associated with the interactions between charged citrate ligands of AuNPs with PANI chains.

We apply PANI@AuNPs and PEDOT@AuNPs for the detection of hydrogen peroxide (H_2O_2) and hypochlorite ions (ClO^-). We reduce the polymer wrapped nanoparticles electrochemically, switch off the potential control and apply portions of H_2O_2 or ClO^- solution. PANI@AuNPs show linear dependence on the concentration of H_2O_2 in the range from 10^{-4} M to 10^{-1} M. Addition of horse radish peroxidase (HRP) enzyme lowers the detection limit from 10^{-4} M to 10^{-8} M. PEDOT@AuNPs show linear response to ClO^- in the range between 10^{-5} and 10^{-3} M. The H_2O_2 or ClO^- detection by PANI@AuNPs or PEDOT@AuNPs by EC-SERS does not require the de-aeration of the supporting electrolyte, what makes this method competitive to other assays.

Keywords: SERS, ROS detection, polyniline, PEDOT, gold nanoparticles, EC-SERS

Figure 1



The scheme of the experimental procedure for H2O2 or ClO- detection.

[Abstract:0247] [Biology/Biomedicine]

Characterization of Molecular Crystals Produced by Microalgae by Means of Raman Microscopy

***Peter Mojzes*[1], *Avital Wagner*[2], *Allen R. Place*[4], *Benjamin A. Palmer*[3]**

[1]*Institute of Physics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic*
[2]*Department of Chemistry, Ben-Gurion University of the Negev, Beer-Sheba, Israel*
[3]*Department of Chemistry, Ben-Gurion University of the Negev, Beer-Sheba, Israel, School of Chemistry, Faculty of Science and Engineering, University of Bristol, Bristol, UK*
[4]*Institute of Marine and Environmental Technology, Center for Environmental Science, University of Maryland, Baltimore, USA*

The recently reported ability of some marine microalgae (e.g., dinoflagellate *Amphidinium carterae*) to form molecular crystals by direct accumulation of diverse N-heterocyclic molecules [Wagner et al., Nat. Biotechnol. 2026, doi: 10.1038/s41587-026-03006-6] has stimulated interest in understanding the molecular mechanisms enabling controlled biocrystallization under conditions where these substances are practically water-insoluble and therefore present in the natural environment only at micromolar concentrations. Given the birefringence and generally high refractive indices of these substances, understanding and technological exploitation of the molecular mechanisms underlying this biocrystallization could lead to the design and production of optical elements for micro- and nano-optics.

Raman microscopy is well-suited for studying the formation of microcrystals inside living cells. It allows determining the chemical composition and polymorphism of molecular crystals *in situ*, without the need for their extraction. Raman microscopy thus conveniently complements the ultrastructural information provided by cryogenic electron microscopy. The most common excitation wavelength for Raman spectroscopy is 532 nm, which allows the acquisition of high-quality spectra not only of crystalline inclusions but also of other biomolecules present in cells, such as lipid droplets, polyphosphate bodies, starch grains, mitochondria, and cell walls.

The current presentation shows that excitations from the visible region are not suitable for studying molecular crystals formed from some pteridines that exhibit strong, persistent autofluorescence. In addition, we show that crystals formed from more soluble substances, such as cytosine or uric acid, often gradually dissolve during the measurement when excited at 532 nm, probably due to slight local heating by the excitation beam. To avoid problems with autofluorescence and thermally induced dissolution of molecular crystals during longer Raman mapping, it is possible to use near-IR excitation, such as 785 nm. However, in the case of molecular crystals of some fluorescent pterins, even excitation at 785 nm was insufficient to suppress undesirable effects. It was the excitation at 830 nm that proved suitable, as it allowed circumventing the problems of autofluorescence, local heating, and cell photobleaching, while also enabling multi-channel detection with standard silicon CCD detectors.

Keywords: molecular crystals, pterins, purines, autofluorescence, Raman microscopy

[Abstract:0248] [Novel Approaches]

Validation of Helicity-Resolved Raman Spectroscopy Using Chiral Testing Materials

***Maria Fernanda Munoz*[1], *Tehseen Adel*[3], *Riccardo Torsi*[1], *Jheng Yi Li*[2], *Saumika Bandopadhyay*[5], *Jeffrey R. Simpson*[4], *Angela Hight Walker*[1]**

[1]*Quantum Measurement Division, National Institute of Standards and Technology, MD, USA*
[2]*Department of Materials Science and Engineering, National Cheng Kung University, Tainan 70101, Taiwan*
[3]*Department of Physical Sciences, University of Findlay, Findlay, OH, USA*
[4]*Astronomy and Geosciences, Towson University, Towson, Maryland USA*
[5]*Department of Physics and Astronomy, Howard University, Washington DC, USA*

To compare data from laboratories around the world, we must reach consensus on terminology and measurands relevant to chiral phonon measurements [1], especially for low-dimensional or 2D materials. Even with linear polarization, errors or artifacts can be seen in published Raman data. Using universally available test materials, methodologies [2], and instrumental parameters, methods have been developed to reduce such issues and enable reproducible results. An effort underway now is to obtain helicity-resolved Raman spectra, including the impact of temperature and excitation wavelength. Our unique magneto-optical measurement capabilities afford diffraction-limited, spatially resolved Raman and photoluminescence measurements while simultaneously varying the polarization (both incident and scattered), temperature (1.6 K to 400 K), laser wavelength (tunability from visible to near-infrared), and magnetic field (up to 9 T). Additionally, coupling to a triple-grating spectrometer provides access to both low-frequency (down to 6 cm-1, or 0.75 meV) phonon and magnon modes and to the spectral resolution required for chiral measurements. By using broadband quarterwave plate (QWP), halfwave plate (HWP) and two polarizers, we can confidently obtain in- or out-phase circularly polarized Raman measurements, allowing us to probe all four combinations: RL, RL, RR and LL, where R and L refer to the handiness right or left, respectively, for the incident or Raman scatter. These four data sets are collected to define a circular intensity difference (CID) which goes beyond intensity changes to observe frequency shifts and permits differentiating the impact of selection rules versus chirality on some test materials, such as α-Quartz (both X- and Z-cut) and Tellurium, as a function of temperature and wavelength of excitation.

References:

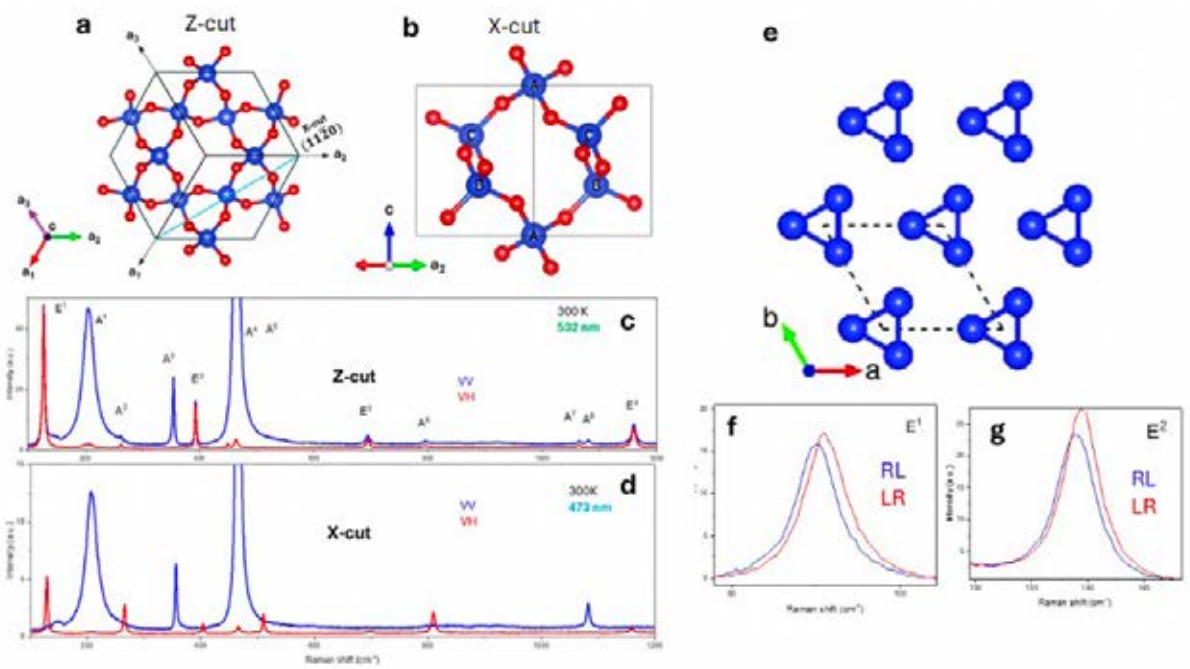
[1] Nature Phys. 2025, 21 1532

[2] Journal of Raman Spectroscopy, 2026,0:1-14

Keywords: methodology, helicity resolved Raman spectroscopy, chiral phonons

Oral Abstracts

Polarized Raman at Room temperature for Testing Materials: Quartz and Tellurium Crystals



(a) Crystal structure for Quartz z-cut and (b) x-cut where blue spheres are SIlicon and red oxygen atoms. b) Phonons at room temperature for z-cut (b) and X-cut (d) under parallel and cross polarization (e) Tellurium crystal structure (f) Helicity resolved Raman for E1 mode and E2 mode (g) under RL and LR polarization.

[Abstract:0253] [Biology/Biomedicine]

Raman Spectroscopic Analysis of Fatty Acid Synthase and Cholesterol Inhibition in Blood Cancers

***Patrycja Dawiec*, Malgorzata Baranska, Katarzyna Majzner**

Department of Chemical Physics, Faculty of Chemistry, Jagiellonian University, Krakow, Poland,

Metabolic flexibility allows hematologic malignancies to rewire lipid pathways. This adaptation supports continued proliferation and promotes survival during therapy stress. Fatty acid synthase (FASN) and cholesterol homeostasis are key metabolic nodes. In lymphoma models, pharmacological inhibition of these nodes can induce swift and varied lipid remodelling.

For lipid-focused research, Raman spectroscopy is preferred for its high sensitivity in detecting lipids in biological samples. In our research, we introduce a Raman-based workflow to monitor lipid pathway disruptions in in vitro lymphoma models. Cells were treated with inhibitors targeting FASN and the cholesterol axis. Single-cell Raman images were processed using a chemometric pipeline to extract concise molecular signatures of lipid remodeling and quantify intracellular heterogeneity. PCA and MCR enabled the detection of changes in cellular biochemical contributions, such as increased lipid uptake from the medium or shifts in lipid fraction composition.

FASN inhibition caused subtype-specific changes in lipid remodeling: Pfeiffer cells accumulated lipids in droplets, while SU-DHL-4 cells primarily consumed these droplets. When exposed to palmitic acid (PA), Pfeiffer cells quickly utilized the supplemented PA, whereas SU-DHL-4 cells mainly stored it in newly formed lipid droplets. Overall, PA supplementation provided exogenous fatty acids that partially compensated for the decrease in endogenous synthesis resulting from FASN inhibition. Concerning the cholesterol pathway, we examined several stages, including the late steps of cholesterol biosynthesis. We observed its uptake and effect through a measurable change in lipid droplet composition.

These findings collectively show that Raman imaging, when paired with chemometrics, can distinguish among different lipid adaptation strategies in hematologic cancer models.

Acknowledgement: This research was funded by the National Science Center Poland (NCN), PRELUDIUM 23 UMO-2024/53/N/ST4/03000.

Keywords: Raman Spectroscopy, Chemometrics, Lipid metabolism

[Abstract:0279] [Coherent Raman Imaging]

Broadband Electronic Resonance Coherent Anti-Stokes/ Stokes Raman Scattering Microscopy for High-Speed and High-Sensitivity Imaging of Biomolecules

***Yusuke Murakami*[1], *Minori Masaki*[2], *Norihide Sagami*[1], *Ikuto Eshima*[1], *Ryosuke Oketani*[1], *Masashi Yanagisawa*[2], *Hideaki Kano*[3], *Sakiko Honjoh*[2], *Kotaro Hiramatsu*[1]**

[1]*Department of Chemistry, Faculty of Science, Kyushu University, Fukuoka, Japan*
[2]*International Institute for Integrative Sleep Medicine (WPI-IIIS), Tsukuba Institute for Advanced Research (TIAR), University of Tsukuba, Ibaraki, Japan*
[3]*Department of Biosciences and Informatics, Faculty of Science and Technology, Keio University, Kanagawa, Japan*

Coherent Raman imaging (CRI) enables label-free visualization of biomolecules in living cells and tissues by detecting their intrinsic vibrational frequencies. Representative CRI techniques provide rapid imaging, molecular specificity, and three-dimensional sectioning capabilities. Despite these advantages, the sensitivity of CRI techniques is typically limited to the millimolar range, making it challenging to visualize low-abundance molecules.

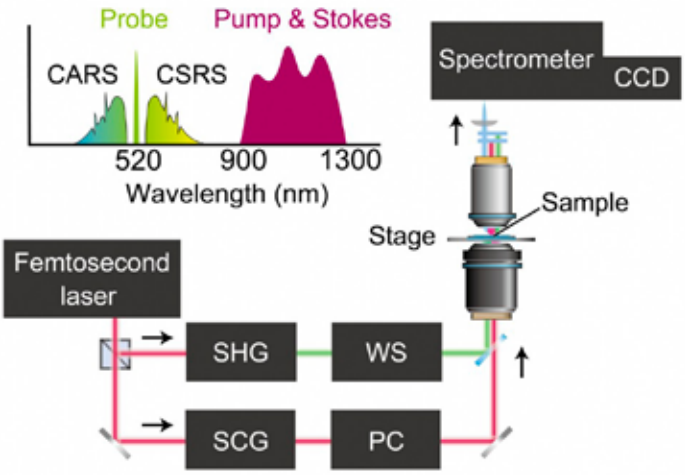
To overcome the sensitivity limit, electronic resonance Raman processes can enhance sensitivity by tuning the excitation wavelength to the electronic absorption band of target molecules. This approach greatly increases the Raman scattering cross section and enables detection down to the sub-micromolar level. However, most implementations rely on narrowband excitation and detection, which limits molecular fingerprinting capability and can lead to ambiguous spectral interpretation due to overlapping signals and non-specific backgrounds such as four-wave mixing and cross-phase modulation, highlighting the need for broadband detection.

In this work, we address these limitations by developing a broadband electronic-resonance coherent anti-Stokes and Stokes Raman scattering (BER-CARS/CSRS) microscopy platform. Our system employs a near-infrared supercontinuum source as the pump and Stokes fields, combined with a narrowband visible laser as the probe field (Fig. 1). This configuration integrates the high sensitivity of electronic resonance with the wide spectral coverage across the fingerprint region.

Using this platform, we achieved label-free cytochrome imaging from live cell organelles to tissues (Murakami et al., bioRxiv, 2025). The cytochrome, endogenous light-absorbing biomolecules, plays a supportive role in the electron transport chain. Figure 2 shows BER-CSRS images of living cells. The bands at 790, 750, and 1010 cm^{-1} are assigned to nucleic acids, cytochromes, and proteins, respectively. In the $Im[\chi(3)]$ spectrum of region (ii) (Fig. 2(b)), a clear peak at 750 cm^{-1} was observed, which originates from cytochromes. Furthermore, the BER-CSRS platform can achieve a frame rate of 2 frames/min using a rapid translational stage for sample positioning (Fig. 2c), suggesting the potential for observing even faster intracellular dynamics. These results indicate the potential of our method for visualizing energy metabolism through cytochrome mapping in life sciences research.

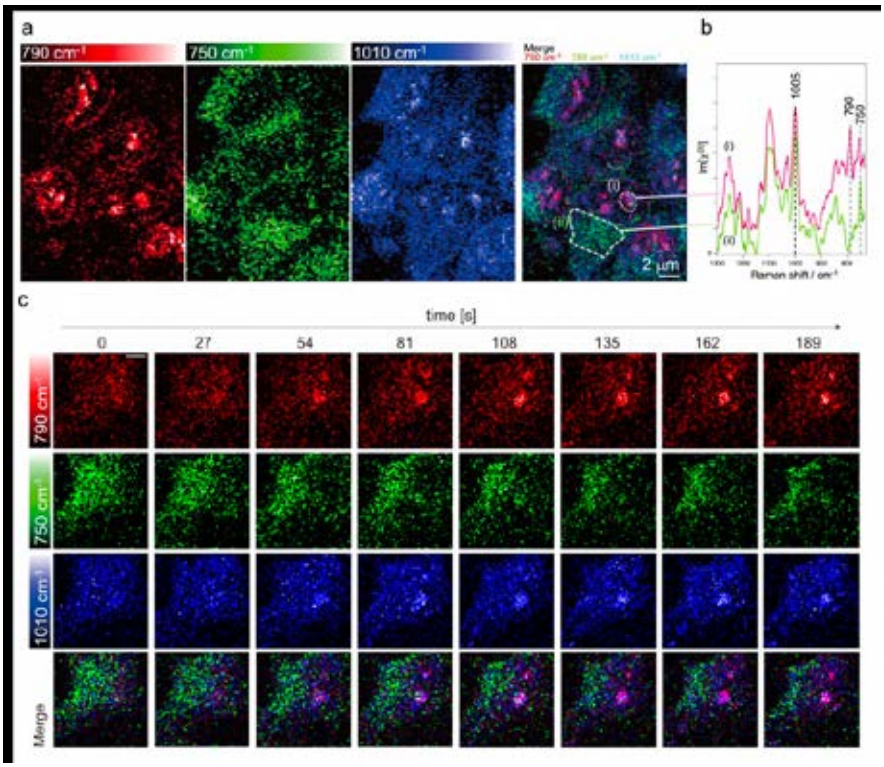
Keywords: coherent Raman imaging, cytochorme, bioimaging,

Figure 1



Schematic of our BER-CARS/CSRS setup. Inset shows spectral profiles of the incident fields and the generated CARS and CSRS fields. SHG: Second harmonic generation, WS: wavelength selector, SCG: supercontinuum generation, PC: pulse compressor.

Figure 2



(a)BER-CSRS images of living HEK293 cells reconstructed at 790 (nucleic acids), 750 (cytochromes) and 1001 cm−1 (proteins). Image size: 101 × 61 pixels, pixel size: 0.5 µm x 0.5 µm, exposure time: 20 ms/pixel. (b) Average Im[$\chi(3)$] spectra corresponding to regions (i) and (ii) in merge image in (a). (c) High speed time lapse BER-CSRS imaging of HeLa cells at 790, 750 and 1010 cm^{-1}. BER-CSRS imaging was initiated at t = 0 s and performed until t = 189 s with a 27-s interval. The image size: 51 × 51 pixels, pixel size: 0.5 µm x 0.5 µm, exposure time: 1 ms/pixel, Scale bar: 5 µm.

[Abstract:0284] [Non-linear/Time-resolved]

Polarization-Resolved Spontaneous Nonlinear Scattering Captures Phonon-Like Motion in Liquids

Masanari Okuno

Department of Basic Science, Graduate School of Arts and Sciences, The University of Tokyo

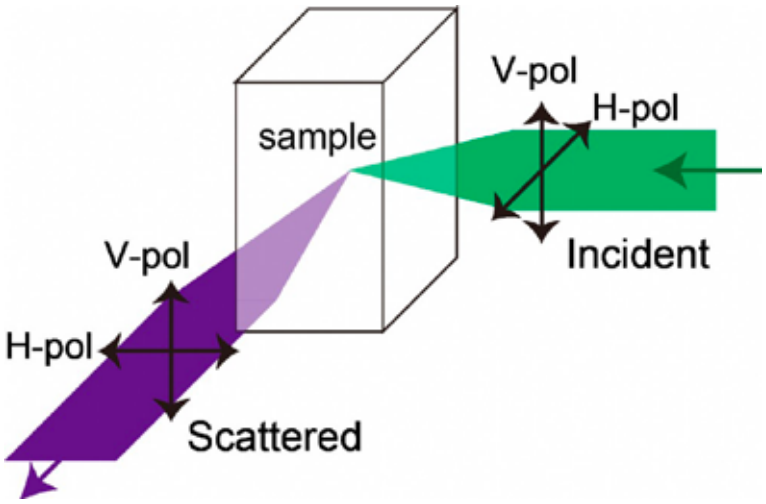
Hyper-Raman and hyper-Rayleigh scattering are nonlinear inelastic and elastic scattering processes, respectively, wherein two photons are absorbed and one photon is emitted. Several studies on liquids using hyper-Raman and hyper-Rayleigh scattering have reported unique polarization-dependent features not observed in Raman spectroscopy. The hyper-Raman/Rayleigh scattering signals from isotropic liquids in the VH and HV polarizations (the first and second letters denote the polarization of the incident and scattered light with respect to the scattering plane, respectively: V: vertical, H: horizontal, see Figure 1) do not coincide. The difference in the spontaneous nonlinear scattering between the two polarization configurations remains unclear. Here, we clarify the polarization dependence using experimental and computational methods.

Figure 2 shows the polarization-dependent hyper-Raman spectra from liquid H2O. The hyper-Raman spectra scattered at 90 degrees are measured by our hyper-Raman spectrometer (J. Phys. Chem. Lett., 14, 3063-3068 (2023), 12, 4780-4785 (2021)). Broad signals ranging from 400 to 1000 cm-1, due to librational modes, and signals around 1650 cm-1, due to the bending mode, are observed. It should be noted that the spectral features in the VH and HV configurations differ significantly, whereas those in the VH and HH configurations agree well. The hyper-Rayleigh scattering signals in the VH(HH) and HV configurations also differ. This contrasts with conventional one-photon excited Raman spectroscopy, where isotropic liquids yield identical signals in the HV and VH configurations.

Molecular dynamics (MD) simulations qualitatively reproduce the polarization dependence of the librational signals in the hyper-Raman spectra from H2O. Namely, the high-frequency librtional band is much larger in the VH(HH) configuration than in the HV configuration. We successfully ascribe this spectral difference to the isotropy of the space-correlation function of the hyperpolarizability tensors across multiple molecules like optical phonon modes. Furthermore, we found that the polarization dependence of hyper-Rayleigh scattering arises from fluctuations in the molecular dipole moment that do not average to zero even on the mesoscopic scale.

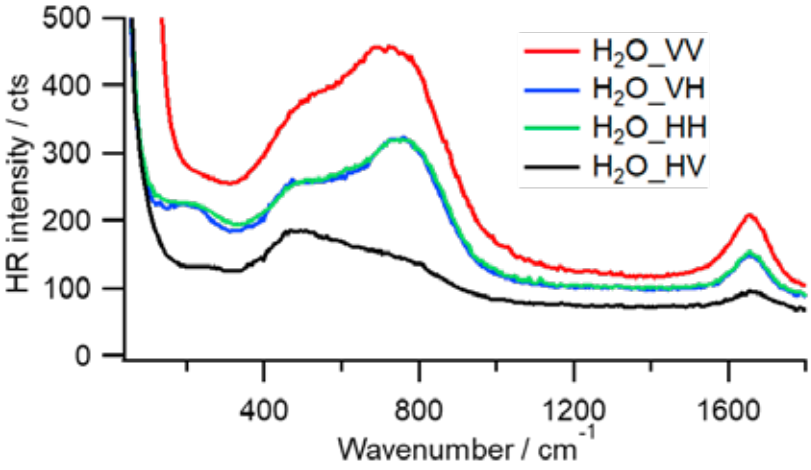
Keywords: Hyper-Raman spectroscopy, Nonlinear Raman spectroscopy, Liquid, Hyper-Rayleigh scattering

Figure1



Polarization configurations of the nonlinear spontaneous scattering

Figure2



Polarization dependence of hyper-Raman spectra from H2O.

[Abstract:0285] [Materials]

Correlative Raman Microscopy Across Disciplines: From Cellular Architecture to 2D Material Heterostructures

***Sabrina Hakelberg**, Ievgeniia Iermak, Ute Schmidt, Miriam Boehmler*

Applications Department, Oxford Instruments WITec, Ulm, Germany

Confocal Raman microscopy combined with complementary imaging modalities enables comprehensive, label-free analysis of heterogeneous samples across both life science and materials research. This contribution presents two scientifically distinct case studies demonstrating how the integration of Raman spectroscopy with widefield, nonlinear optical, and topographic techniques enhances our understanding of complex structure-property relationships.

In the first example, multimodal analysis is applied to biological specimens including cells, tissues, and subcellular structures (figure 1a+b). Three-dimensional Raman imaging reveals biochemical composition with high spatial precision, while second- and third-harmonic generation (SHG/THG) imaging provide structural information on collagen-rich tissue and refractive index interfaces. Correlation with fluorescence, white-light imaging, and complementary topographic methods enables direct linking of molecular signatures with morphology, mechanical properties, and metabolic states. These results highlight how multimodal microscopy approaches support non-destructive characterization of biological specimens.

The second case study focuses on heterostructures composed of MoS_2 and WS_2, covered with a graphene sheet (figure 1c+d). Raman, photoluminescence (PL), and polarization-resolved second-harmonic generation imaging are used to investigate strain fields, defect distributions, resonant exciton-phonon interactions, and interlayer coupling phenomena. High-resolution Raman imaging distinguishes monolayers, bilayers, and overlapping regions, while PL imaging reveals exciton energy shifts associated with local stacking configurations. SHG measurements identify grain orientations and symmetry variations within the heterostructure.

Together, these examples illustrate how confocal Raman microscopy combined with nonlinear optical and topographic imaging provides a unified framework for resolving chemical, structural, and optical properties across diverse classes of materials. The ability to integrate multiple contrast mechanisms within a single analytical instrument enables researchers to address a wide range of questions, from biological specimen to interlayer coupling in 2D heterostructures. Having all data in one software enables easy and straightforward correlation of results. Such methodological versatility, combined with the need to accommodate users from different scientific backgrounds, makes this type of multimodal instrumentation particularly well suited for core facilities, where a robust, adaptable, and broadly applicable platform is essential.

Keywords: Raman spectroscopy, Confocal imaging, Correlative, Life Science, 2D Materials

Multimodal Imaging of Lung Carcinoma Cells and 2D Heterostructures

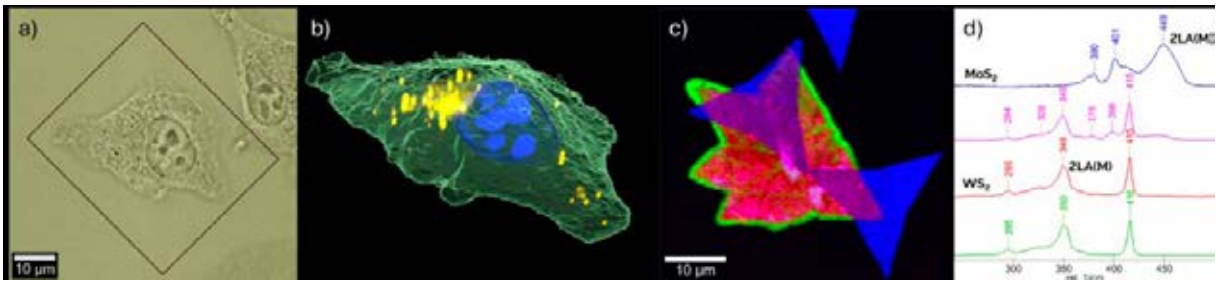


Figure 1: a) Brightfield image of a lung carcinoma epithelial cell in cell culture. b): False colour-coded 3D Raman image of a cell generated from the hyperspectral data set. Nucleoli in blue, cytoplasm in green and vesicles in yellow. c) False colour-coded Raman image of the 2D heterostructure revealing structural details, with corresponding Raman spectra in d).

[Abstract:0286] [SERS/TERS/Plasmonics]

SERS-Based Detection of Cancer Cell Surface Proteins for Early Cancer Diagnosis

***Eungyeong Park*[1], *Ju Hyun Park*[2], *Young Mee Jung*[3]**

[1]*Kangwon Radiation Convergence Research Support Center, Kangwon National University, Chuncheon 24341, Korea*
[2]*Department of Biomedical Science, Kangwon National University, Chuncheon 24341, Korea, Institute for Molecular Science and Fusion Technology, Kangwon National University, Chuncheon 24341, Korea*
[3]*Kangwon Radiation Convergence Research Support Center, Kangwon National University, Chuncheon 24341, Korea, Institute for Molecular Science and Fusion Technology, Kangwon National University, Chuncheon 24341, Korea, Department of Chemistry, Kangwon National University, Chuncheon 24341, Korea*

Surface-enhanced Raman scattering (SERS) has emerged as a powerful analytical technique for the highly sensitive detection of biomolecules due to its molecular fingerprint specificity and strong signal enhancement capability. In particular, the detection of cancer-related biomarkers at the cellular level has attracted significant attention for early diagnosis and monitoring of tumor progression.

First, we developed an antibody-conjugated SERS immunoassay platform based on silica-coated gold nanoparticles for the selective detection of epithelial cancer markers such as EpCAM and E-cadherin in both fixed and living cells. This platform enables in situ and quantitative detection of cell surface proteins at the single-cell level without destructive sample preparation. [Biosens. Bioelectron. 2023, 234, 115366.]

Second, a SERS immunoassay platform employing core–shell structured magnetic gold nanoparticles was designed for sensitive detection of circulating tumor cells. The engineered nanostructure generates dense electromagnetic hotspots, significantly enhancing Raman signals and enabling multiplex detection of target proteins. This platform allows highly sensitive, quantitative analysis of multiple protein biomarkers and represents a promising tool for advancing precision diagnostics and personalized therapeutic strategies in breast cancer management.

Furthermore, these SERS nanoprobe platforms demonstrate the strong potential of SERS-based analytical approaches for sensitive and multiplexed detection of cancer biomarkers.

Keywords: Surface-enhanced Raman scattering (SERS), SERS immunoassay, Multiplex biomarker detection

[Abstract:0287] [Novel Approaches]

Plasmonic Microspheres in Flow: Acoustofluidic Focusing for Sensitive SERS Detection

***Vít Pavelka*, Lucie Březinová, Jakub Novotný, Jan Přikryl, Michal Javorek, Anna Týčová**

Institute of Analytical Chemistry of the Czech Academy of Sciences, v. v. i., Brno 602 00, Czech Republic

Integrating colloidal surface-enhanced Raman spectroscopy (SERS) substrates into microfluidic analytical systems remains a challenging task. Although solid substrates provide structural stability, their performance is often limited by insufficient analyte residence times and restricted mass transport. Plasmonic colloids represent a more suitable alternative, but their use requires both stabilization in complex media and efficient concentration at the probed region. Both limitations can be mitigated by immobilizing nanoparticles onto larger carrier structures.

Here, we present a strategy for the synthesis and acoustofluidic manipulation of silver-decorated polystyrene microspheres (PS-AgNPs), designed as mobile SERS-active carriers for in-flow Raman detection. The system was transitioned from commercially available PS microspheres (~5 μm) to fully in-house synthesized PS (~1–5 μm) and AgNPs (~40 nm). The immobilization of AgNPs onto the polystyrene carriers is facilitated by residual polymeric stabilizers present on the surface, enabling rapid nanoparticle attachment without additional chemical surface modification and ensuring controllable surface coverage.

The resulting composites exhibit strong plasmonic activity and uniform SERS performance. Raman mapping experiments performed on individual microspheres, using adenine and thiamine as model analytes, revealed homogeneous signal distributions with coefficients of variation below ~10 % and limits of detection reaching 100 nM for adenine. The reported performance corresponds to ~5μm microspheres. Preliminary results further demonstrate successful preparation and manipulation of ~1μm PS-AgNPs under flow conditions, with expected improvements in effective SERS-active surface density. Representative SEM image and SERS intensity map confirming the localized signal response are shown in Figure 1.

To evaluate substrate performance, we implemented a software-driven workflow for automated and quantitative analysis of nanoparticle coverage and SERS efficiency across large datasets.

For in-flow concentration of PS-AgNPs, an acoustofluidic approach was employed, enabling their continuous manipulation. In capillary-based systems, particle focusing in the channel centre resulted in stable and reproducible SERS detection under flow conditions.

Ongoing work focuses on the development of a microfluidic chip for acoustofluidic separation of PS-AgNPs from free AgNPs. These developments are expected to advance Raman imaging and detection of biologically relevant molecules in flowing microenvironments.

Keywords: SERS, acoustofluidics, plasmonic microspheres, in-flow detection, particle focusing, Raman mapping

Figure 1

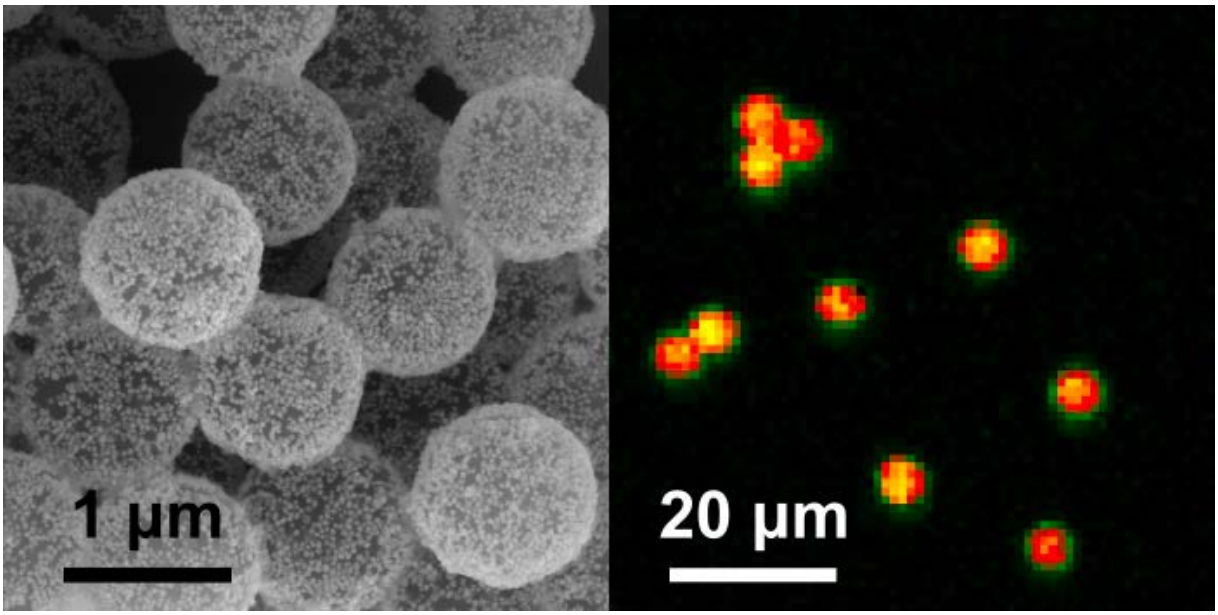


Figure 1. (left) SEM image of PS-AgNPs with a diameter of ~1 µm. (right) SERS intensity map obtained from ~5µm PS-AgNPs by integrating the adenine band (~732 cm^{-1}) after automated baseline correction. The microspheres were incubated with 500 nM adenine solution, purified, and immobilized on a silicon substrate prior to measurement.

[Abstract:0290] [SERS/TERS/Plasmonics]

Angularly Resolved Raman Spectroscopy of Cobalt(II) Phtalocyanine Through a Particle on Mirror System

***David Baschnagel*[1], *Daniel Schäfer*[2], *Felix Schneider*[1], *Alfred J. Meixner*[1], *Sebastian Schlücker*[2], *Dai Zhang*[1]**

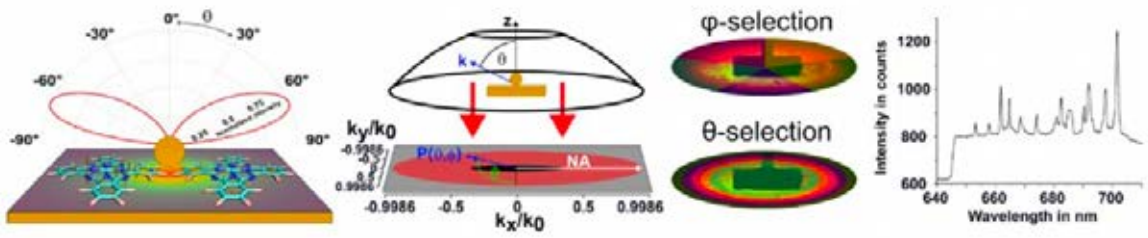
[1]*Institute for Physical and Theoretical Chemistry, Eberhard Karls University Tübingen, Germany*
[2]*Physical Chemistry I, Department of Chemistry and Center of Nanointegration Duisburg- Essen, Germany*

Surface-enhanced Raman scattering (SERS) has become a widely used technique in the chemical sciences. Typically, substrates composed of metallic nanostructures are employed for SERS, as these can elicit electromagnetic enhancement due to robust plasmon resonance. For the system of gold nanospheres on a mirror, several resonances have been identified, which exhibit distinct plasmonic properties. Theoretical work predicts that the emission behavior of the individual resonances also differs. The objective of this study is to angularly resolve the Raman signal in order to elucidate its spatial distribution in the k-space. Through the application of various electric field distributions in the focus the interaction of directional Raman scattering and plasmonic resonances was investigated.

The fabrication of gold nanosphere-on-mirror samples entailed the drop-casting of super spherical gold nanoparticles onto a substrate comprising an ultra-smooth gold film and a cobalt(II) phthalocyanine (CoPc) layer. When exposed to a cw laser radiation of 633 nm or 785 nm, the resulting system exhibits multiple resonances, with two occurring at approximately 600 nm and 800 nm, respectively. Both resonances were investigated with radial and azimuthal polarization to excite the system with an electric field direction both perpendicular and parallel to the sample plane. To obtain information about the spatial distribution of the Raman signal, the back focal plane was divided into angular ranges from which energy momentum spectroscopy was performed. The findings suggest a correlation between the Raman scattering of CoPc and the radiation behavior of the plasmonic resonances. A comparison of the angular distribution of gold photoluminescence and Raman scattering reveals fundamental differences between them. The variation of the excitation field directions and the excitation wavelengths results in strong directional changes in the angular Raman scattering behavior.

Keywords: Surface-enhanced Raman scattering, plasmon resonance, energy momentum spectroscopy

Figure 1



a) Simulated θ-plot emission of a gold nanosphere on CoPc. b) Collection sketch of the parabolic mirror. c) Illustration of the segmentation in the k-space. d) Example of a SERS spectrum collected in an angular segment.

Oral Abstracts

[Abstract:0291] [Materials]

Metrological Calibration of Raman Shift for Strain Quantification in 4H-Silicon Carbide

***Nasim Zarrabi*[1], *Cameron Wilson*[4], *Ben Breeze*[2], *Gloria Zhao*[2], *Mark Senn*[4], *Vishal Shah*[3], *Ben Green*[2], *Sebastian Wood*[1]**

[1]*Electrochemical and Electromagnetic Technologies Department, National Physical Laboratory, Teddington, UK*
[2]*Physics Department, University of Warwick, Coventry, UK*
[3]*School of Engineering, University of Warwick, Coventry, UK*
[4]*Chemistry Department, University of Warwick, Coventry, UK*

Raman spectroscopy is widely used for strain measurements in semiconductor materials because it is sensitive to lattice distortions, offers high spatial resolution, and is fully non destructive. However, Raman peak shifts cannot directly provide absolute strain values without a proper calibration that links the spectral changes to the actual lattice deformation. Strain plays a critical role in semiconductor behaviour by affecting electrical properties, influencing defect formation, and ultimately altering device performance. Creating a reliable calibration curve is therefore an important methodological step, enabling Raman spectroscopy to be used as a practical and non destructive tool for quantifying strain arising from semiconductor material growth and device fabrication. In this work, we establish such a calibration curve for the 4H polytype of silicon carbide (SiC), a technologically important wide bandgap semiconductor that is increasingly used in high power, high temperature, and high frequency electronic devices. The ability of SiC to operate under harsh conditions makes it essential for electric vehicles, power conversion systems, and emerging energy technologies, but its performance is strongly linked to controlling strain and defects within the crystal lattice.

The methodology combines diamond anvil cell (DAC) hydrostatic compression with Raman spectroscopy and X ray diffraction (XRD). Hydrostatic strain was applied in controlled, sequential pressure steps by compressing SiC samples inside the DAC, ensuring uniform deformation of the lattice. Raman spectra were recorded at each pressure increment to monitor the evolution of SiC phonon modes. In parallel, XRD was used to obtain direct, quantitative, and SI-traceable measurements of lattice spacing under the same hydrostatic loading conditions. By correlating Raman peak positions with XRD derived strain values at each pressure step, we constructed a robust calibration curve that links Raman spectral shifts directly to hydrostatic strain in SiC. This calibration offers a practical pathway for using Raman spectroscopy as a stand alone, non destructive technique for strain quantification in SiC materials and devices, supporting improved process monitoring and reliability assessment.

Keywords: Raman Spectroscopy, Metrology, Semiconductor Materials, Silicon Carbide

[Abstract:0293] [Novel Approaches]

qRICO-Net: Machine-Learning-Based Crystallographic Orientation Mapping Using Polarized Raman Microscopy

***Andrii Kutsyk*[1], *Danylo Komisar*[1], *Konstantinos Stergiou*[1], *Yurii Pilhun*[1], *Stela Canulescu*[2], *Evgeniia Gilshtein*[2], *Daniel Abou-Ras*[3], *Oleksii Ilchenko*[1]**

[1]*Lightnovo ApS, Birkerød 3460, Denmark*
[2]*Department of Electrical and Photonics Engineering, Technical University of Denmark, Roskilde 4000, Denmark*
[3]*Department for Structure and Dynamics of Energy Materials, HelmholtzZentrum Berlin fur Materialien und Energie GmbH, Berlin 14109, Germany*

Quantitative Raman Imaging for Crystal Orientation analysis (qRICO) is capable of performing fast, simple orientation mapping of materials using polarized Raman microscopy and image reconstruction [1]. It is a non-destructive, cost-effective, and fast characterization technique for 2D and 3D orientation mapping of polycrystalline materials with no sample preparation requirements. The basic idea involves the simultaneous measurement of Raman scattering at different polarization setups (16 polarization channels).

qRICO requires knowledge of the Raman tensor elements and, for optically anisotropic systems, measurement of the corresponding Jones matrices, resulting in more complex analytical expressions [2]. qRICO-Net is a way to face these challenges indirectly using data-driven approach. Polarized Raman measurements were correlated with crystallographic orientation maps obtained by EBSD, which served as ground truth for training. qRICO-Net takes a per-pixel spectra and applies 2D convolutions over polarization and wavenumber to extract a spectral feature embedding. The features are globally pooled and passed through residual MLP blocks to regress a 6D rotation representation, which is converted into an SO(3) rotation matrix for symmetry-aware misorientation loss. This design separates spectral feature learning from physically consistent orientation regression. The model was tested using Sb2S3 samples (Fig. 1). Sb2S3 is a quasi-1D solar absorber whose solar cell performance strongly depends on crystallographic orientation, where grains oriented close to the [hk1] direction promote favorable charge-transport pathways and reduce recombination losses. The orientations predicted with qRICO-Net (Fig. 1E) are in good agreement with EBSD results (Fig. 1F) with an average misorientation angle of 9 degrees. A successful data-driven qRICO could become the key orientation mapping tool for various functional, polycrystalline thin films in optoelectronic devices, and enable systematic optimization of the absorber microstructure to improve solar-cell efficiency.

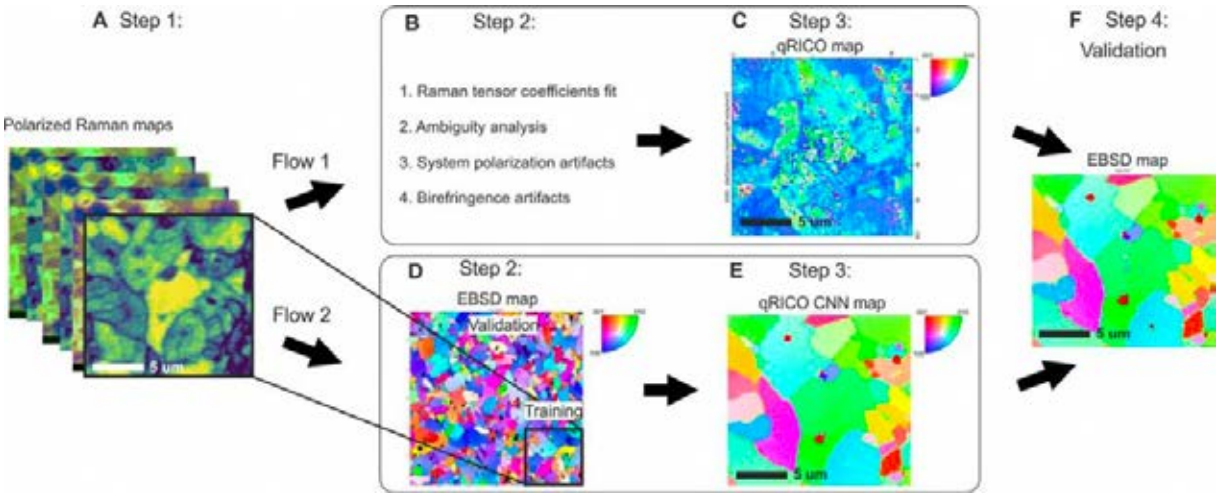
References:

[1] Ilchenko O. et al., Fast and quantitative 2D and 3D orientation mapping using Raman microscopy, Nat. Commun. 2019, 10, 5555.

[2]. Kranert C. et al., Raman Tensor Formalism for Optically Anisotropic Crystals. Phys. Rev. Lett. 2016, 116, 1.

Keywords: polarized Raman microscopy, machine learning, solar cells, orientation mapping

Figure 1



(A) qRICO maps of Sb2S3 films, (B) illustration of analytical steps that must be conducted, (C) orientation map obtained by qRICO of the same area as shown on Fig. 1F. The colors refer to the orientations as defined by the inverse pole figure (top right), (D) EBSD map used for training and validation, (E) orientation map obtained by qRICO-Net, (F) orientation map obtained by EBSD.

[Abstract:0298] [Materials]

High-Temperature Raman Imaging: Unveiling Mineral Processes in Refractory and Ceramic Materials

***Sinje Zimmer*, Kerstin Hauke**

Forschungsgemeinschaft Feuerfest e. V.

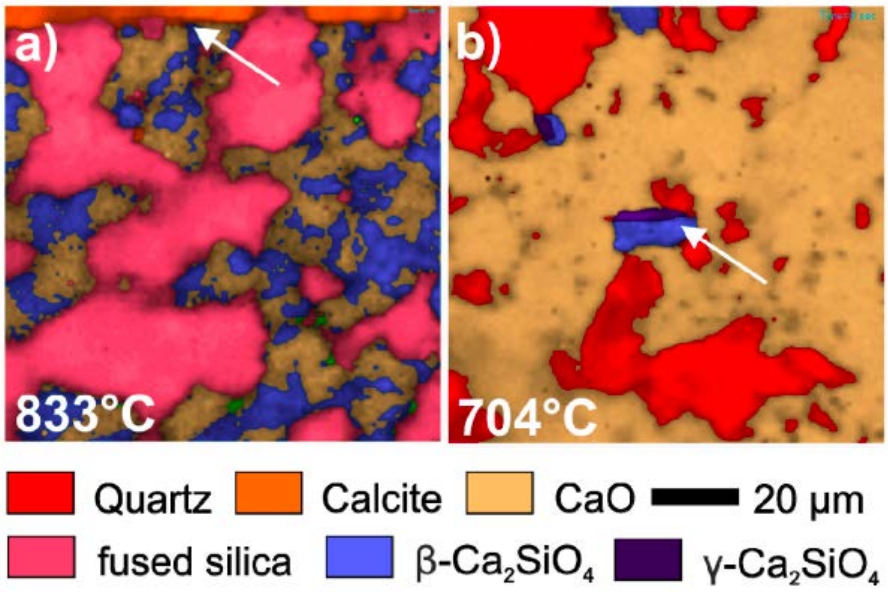
High-temperature Raman imaging is a unique method for analyzing the kinetic behavior of refractory and ceramic materials under extreme thermal conditions. This technique enables in situ, spatially resolved monitoring of phase transformations, kinetic processes, and microstructural changes at temperatures up to 1500°C. Additionally, it allows for the observation of critical intermediate phases.

In this talk, we demonstrate how high-temperature Raman imaging can be used to track the evolution of key phases and reaction kinetics in refractory and ceramic systems. For example, in a calcite-kaolinite sample, we were able to track the decarbonization of calcite to CaO. Additionally, in a green body containing quartz, alkali feldspar, kaolinite, and calcite, we detected pseudowollastonite at ~1125°C, ~290°C below the accepted critical temperature for the transformation of wollastonite to pseudowollastonite.

Visualizing and analyzing dynamic processes directly enhances our understanding of high-temperature reactions and supports the development of advanced refractory and ceramic materials.

Keywords: HTRI, in situ, high-temperature, Raman Imaging, refractory, ceramics

High-temperature Raman Imaging



Hyperspectral Raman images of (a) fused silica-calcite and (b) quartz-lime green bodies recorded at 833 and 704°C with a total exposure time of about 2 h, showing line-by-line image shifts. The sudden phase changes (white arrows) indicate that the respective reactions in (a), i.e., CaCO3 → CaO + CO2↑, and (b), i.e., γ-Ca2SiO4 → β-Ca2SiO4, were faster than the total imaging time.

[Abstract:0302] [Materials]

Water-Vapor İnduced Crystal Transformation from the Jahn-Teller Rb_2CuCl_4 to the Pseudo Jahn-Teller $Rb_2CuCl_4(H_2O)_2$: Diffusion Dynamics Study

***Luis Gómez Fernández*[1], *Fernando Rodriguez*[2], *Fernando Aguado Menéndez*[2], *Rafael Valiente*[1]**

[1]*Department of Applied Physics, Faculty of Sciences, University of Cantabria, 39005 Santander, Spain*
[2]*Department of Earth Sciences and Condensed Matter Physics (DCITIMAC), Faculty of Sciences, University of Cantabria, 39005 Santander, Spain*

This work investigates the hydration of the Jahn-Teller (JT) compound Rb_2CuCl_4 to the Pseudo-Jahn-Teller compound $Rb_2CuCl_4(H_2O)_2$ [F. Aguado et al, Physical Review B 70 (2004) 214104

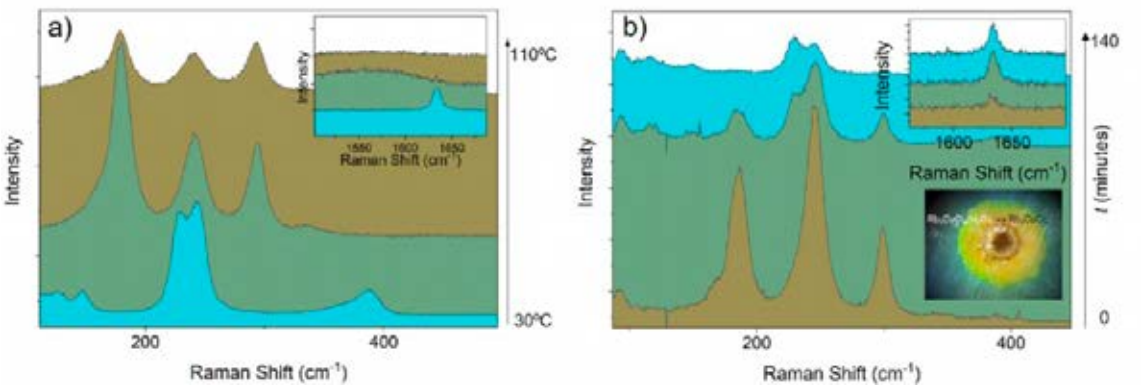
390, M. J. Riley et al, Inorganic Chemistry 27 (1988) 1924] under an enriched vapor environment. The process was studied experimentally using Raman spectroscopy, which provides a clear spectral signature for both phases [L. Gómez et al, Physical Review B 112 (2025) 174117]. The hydration dynamics depend strongly on the wavelength of the laser probe, primarily due to the intrinsic optical absorption of each phase, which can locally influence both hydration and dehydration kinetics. In parallel, the dehydration of $Rb_2CuCl_4(H_2O)_2$ was examined using a heating stage up to 110 ºC. Taking advantage of the optical transparency window defined by the Cl^- to Cu^{2+} charge-transfer and Cu^{2+} (3d9) intraconfigurational transitions, we employed the 514.5 nm and 532 nm excitation lines as probes, as laser-induced heating is minimized in this range. In contrast, red (647 nm) or infrared (785 nm) lines lead to significant sample heating and trigger a local structural transformation from the hydrate to the anhydrous crystal (see figure).

Both forward and reverse processes– Rb_2CuCl_4 - $Rb_2CuCl_4(H_2O)_2$–were studied under controlled vapor atmospheres (Fig. 1). Raman spectra were use to determine the relative fractions, enabling the development of a diffusion model from which to describe the transformation kinetics. Notably, due to the distinct absorption characteristics of two crystals, a pronounced thermochromic effect is observed across this reversible reaction.

Financial support from Project PID2025-171627NB-I00, from the State Research Agency of Spain, Ministry of Science and Innovation and from Project VQ17 (Contrato Programa Gobierno de Cantabria–Universidad de Cantabria) is acknowledged.

Keywords: Pseudo Jahn-Teller effect, Structural phase transition, Vibrational states, Layered crystals, Metal halides, Single crystal materials

Fig. 1



a) Raman spectrum of the compound Rb2CuCl4(H2O)2 as a function of temperature. At approximately 75 °C, the compound undergoes dehydration, transforming from Rb2CuCl4(H2O)2 to Rb2CuCl4. b) Raman spectrum of Rb2CuCl4 as a function of time under a controlled water-vapor atmosphere. As time progresses, the compound gradually transforms into Rb2CuCl4(H2O)2. An optical image of the sample after degradation by the laser probe is also shown, revealing a fully dehydrated central region surrounded by a rehydrated area.

[Abstract:0303] [SERS/TERS/Plasmonics]

SERS-Based Drug Monitoring and Biomarker Detection in Complex Biological Matrices

***Dana Cialla-May*[1], *Juergen Popp*[2]**

[1]*Leibniz Institute of Photonic Technology, Member of Leibniz Health Technologies, Member of the Leibniz Centre for Photonics in Infection Research (LPI), Jena, Germany*
[2]*Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich Schiller University Jena, Member of the Leibniz Centre for Photonics in Infection Research (LPI), Jena, Germany*

Surface-enhanced Raman spectroscopy (SERS) has emerged as a powerful analytical tool for biomedical and bioanalytical applications owing to its exceptional molecular specificity and trace sensitivity. [1] In this contribution, clinically relevant SERS-based strategies for the detection of drugs and biomarkers are presented, demonstrating the potential of advanced plasmonic substrates combined with machine learning data analysis approaches for biomedical diagnostics.

We report silver dendritic nanostructures that provide trace sensitivity and long-term stability, enabling therapeutic drug monitoring in blood plasma. [2] Sulfate ions act as growth-directing and mild capping agents, resulting in passivated metallic surfaces with enhanced resistance to oxidation and signal degradation, as confirmed by SEM, TEM, XRD, and XPS analyses. The substrates enable sub-femtomolar detection of 4-mercaptobenzoic acid and retain stable SERS performance for more than seven months under ambient storage conditions. Following methanol-based protein precipitation, sensitive detection of clinically relevant drugs, such as 6-thioguanine, methotrexate, erlotinib, doxorubicin, and moxifloxacin, in human blood plasma was achieved, with limits of detection within therapeutically relevant concentrations. These results highlight the suitability of the developed substrates for quantitative analysis in clinically relevant matrices.

Beyond drug monitoring, we explored SERS for non-invasive biomarker detection in human cerumen. Multimodal vibrational spectroscopic analysis combining Raman, SERS, coherent anti-Stokes Raman scattering (CARS), stimulated Raman scattering (SRS), and optical photothermal infrared spectroscopy revealed lipids and proteins as the dominant constituents and emphasized the diagnostic potential of cerumen as an easily accessible biofluid. [3] Coupling SERS measurements with machine-learning analysis (PCA–LDA) enabled rapid screening for head and neck cancer, achieving a classification accuracy of 87.2%, highlighting the potential of SERS-based approaches for rapid, minimally invasive clinical diagnostics. [4]

Acknowledgement: The Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) supported this work under grant 465289819.

Literature:

[1] D. Cialla-May et al., Chem. Soc. Rev., 53, 8957-8979 (2024).

[2] A. Dwivedi et al., Advanced Science (2026), online: 10.1002/advs.202517092.

[3] E. Farnesi, M. Calvarese et al., Analyst, 149, 5381-5393 (2024).

[4] E. Farnesi et al., npj Biosensing, 2, 14 (2025).

Keywords: SERS, drug molecules, biomarker, complex biological matrix

Oral Abstracts

[Abstract:0306] [Non-linear/Time-resolved]

Initial Phase of Bimolecular Reactions Between P-Terphenyl Derivatives and Carbon Tetrachloride Detected by Picosecond Time-Resolved Raman Spectroscopy

Mao Tanaka, Shunrou Tokonami, Koichi Iwata

Department of Chemistry, Gakushuin University, Tokyo, Japan

Several aromatic molecules, including *p*-terphenyl, react with carbon tetrachloride (CCl_4) when they are excited to the first excited singlet (S_1) state. The trichloromethyl (CCl_3) radical has been detected as a common reaction intermediate in these reactions, indicating that the excited aromatic molecules extract a Cl radical as the first step of the photochemical process. The aromatic molecules in their S_1 state and carbon tetrachloride are therefore regarded as reactants in a bimolecular reaction in solution. The kinetics of this bimolecular reaction can be monitored by time-resolved spectroscopy without being hindered by diffusion of the reactants if an aromatic molecule is photoexcited in a carbon tetrachloride solution, where the reactant carbon tetrachloride is always located next to the aromatic molecule.

We previously observed mode-selective acceleration of vibrational dephasing in the S_1 state of *p*-terphenyl in carbon tetrachloride (Iwata, *J. Raman Spectrosc.*, 2008). The acceleration of vibrational dephasing for these vibrational modes most likely reflects the bimolecular reaction between S_1 *p*-terphenyl and carbon tetrachloride that proceeds in 5.6 ps. The vibrational modes of highly symmetric *p*-terphenyl, however, are mostly delocalized over the entire molecule. It was difficult to discuss the specific location in the S_1 *p*-terphenyl molecule where the vibrations are suddenly disrupted by the collision that initiates the bimolecular reaction.

In the present study, we examine the photochemical reactions between six *p*-terphenyl derivatives and carbon tetrachloride. Their pseudo-first order rate constants are determined by picosecond time-resolved fluorescence spectroscopy, while the S_1-state Raman spectra, measured with a highly stable time-resolved Raman spectrometer (Tokita, Takaya, Iwata, *J. Raman Spectrosc.*, 2021), reveal broadening of Raman bands only for a few vibrational modes. This result suggests a mode-selective acceleration of vibrational dephasing in the *p*-terphenyl derivatives upon collision with carbon tetrachloride, which initiates the reaction.

Keywords: time-resolved Raman, bimolecular reaction, vibrational dephasing

[Abstract:0307] [SERS/TERS/Plasmonics]

Deep Learning Analysis of Individual DNA Dynamics on A Nanoparticle by Single-Molecule SERS Spectra

***Kuo Zhan*[1], *Peilin Xin*[1], *Zuyan Chen*[3], *Yingqi Zhao*[1], *Han Gu*[5], *Zongyu Wu*[5], *Zhou Chen*[5], *Mulusew W Yaltaye*[2], *Viktorija Pankratova*[4], *Shuai Li*[3], *Jian Ye*[5], *Jianan Huang*[1]**

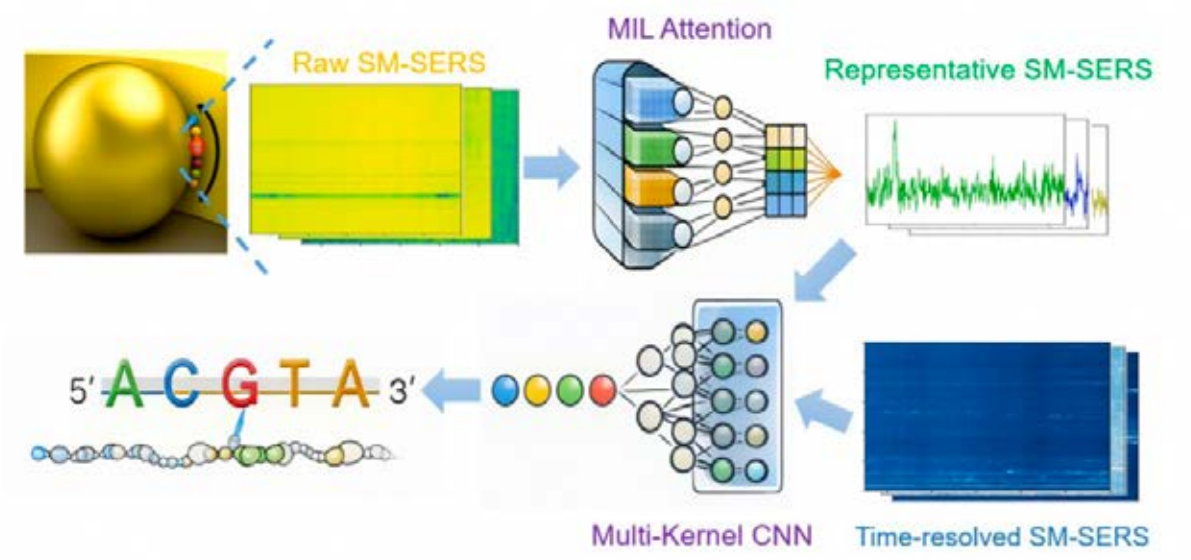
[1]*Research Unit of Health Sciences and Technology, Faculty of Medicine, University of Oulu, 90220 Oulu, Finland; Biocenter Oulu, University of Oulu, 90220 Oulu, Finland*
[2]*Research Unit of Disease Networks, Faculty of Biochemistry and Molecular Medicine and Biocenter Oulu, University of Oulu, 90220 Oulu, Finland*
[3]*The Biomimetics and Intelligent Systems (BISG) research unit, Faculty of Information Technology and Electronic Engineering, University of Oulu, 90220 Oulu, Finland*
[4]*Nano and Molecular Systems Research Unit, Faculty of Science, University of Oulu, 90570 Oulu, Finland*
[5]*State Key Laboratory of Systems Medicine for Cancer, School of Biomedical Engineering, Shanghai Jiao Tong University, Shanghai, People's Republic of China*

Single-molecule surface-enhanced Raman spectroscopy (SM-SERS) measurements are often complicated by stochastic spectral fluctuations arising from molecular motion, variable adsorption configurations, and orientation changes on metallic surfaces. In our previous work, we developed a particle-in-well (PIW) plasmonic platform, which enables long-term, stable SM-SERS measurements of individual DNA molecules on a gold nanoparticle. However, DNA oligomers adsorbed on the gold nanoparticle surface exhibit pronounced spectral fluctuations due to changes in molecular orientation and diffusion. As a result, time-resolved SM-SERS spectra often display stochastic "jumping" behavior, making conventional peak-based analysis subjective, unstable, and difficult to generalize.

Here, we introduce a data-driven framework combining Multiple Instance Learning (MIL) and a multi-kernel convolutional neural network (CNN) for the interpretation of time-resolved SM-SERS spectra acquired from the PIW platform. Rather than relying on manually selected spectral peaks, the framework learns discriminative SM-SERS spectral representations directly from large collections of dynamic SM-SERS spectra. Using this approach, we investigated ten DNA heptamers with different base compositions and sequence patterns. By constructing positive–negative spectral combinations, the MIL framework enabled the extraction of representative SM-SERS spectral groups, including citrate background spectra, base-dominant classes (A-, C-, G-, and T-dominant), and binary base-combination classes. The multi-kernel CNN trained on these 15 representative SM-SERS spectral groups achieved an overall classification accuracy exceeding 88%. The trained model was further applied to analyze time-resolved SM-SERS spectral trajectories of known DNA oligomers, enabling dynamic identification and comparison of their sequence-dependent SM-SERS spectral behaviors on the gold nanoparticle surface, with a focus on the single-molecule spectral identification and interpretation of short DNA chains. More broadly, the combination of PIW single-molecule sensing and Data-driven deep learning analysis provides a robust framework for studying sequence-dependent SM-SERS spectral dynamics and offers future potential for sequencing-related biomolecular SERS spectra analysis.

Keywords: Single-molecule SERS, DNA oligomers, Multiple instance learning, Deep learning, Spectral dynamics

Graphic abstract: Data-driven analysis pipeline for SM-SERS dynamics on a particle-in-well (PIW) platform.



Single-molecule surface-enhanced Raman scattering (SM-SERS) signals are first acquired from DNA oligomers interacting with a gold nanoparticle in the PIW system. The raw time-resolved SM-SERS spectra are processed using a multiple-instance learning (MIL) attention framework, which identifies and selects representative spectra from highly heterogeneous single-molecule spectral streams. These representative SM-SERS spectra are then used to train a multi-kernel convolutional neural network (CNN) model capable of capturing spectral features across different Raman shift scales. The trained model subsequently enables direct prediction and classification of short DNA oligomers from time-resolved SM-SERS measurements, facilitating dynamic identification and comparison of sequence-dependent spectral behaviors of DNA bases on the gold nanoparticle surface.

[Abstract:0310] [Biology/Biomedicine]

Spectral Signature of Hypoxia. Time-Dependent Effects on Brain Endothelium Revealed by FTIR and Raman İmaging

***Aleksandra Pragnąca*[1], Natalia Warchoł[2], Zuzanna J. Krysiak[3], Anna Antolak[2], Robert Zdanowski[3], Kamilla Malek[2]**

[1]*Faculty of Chemistry, Department of Chemical Physics, Raman Imaging Group, Jagiellonian University, Krakow, Poland; Doctoral School of Exact and Natural Sciences, Jagiellonian University, Krakow, Poland*
[2]*Faculty of Chemistry, Department of Chemical Physics, Raman Imaging Group, Jagiellonian University, Krakow, Poland*
[3]*Military Institute of Medicine - National Research Institute, Laboratory of Molecular Oncology and Innovative Therapies, Warsaw, Poland*

Brain endothelial cells, essential components of the blood-brain barrier, are particularly vulnerable to stress during neurodegenerative processes. Hypoxia, a hallmark of these conditions, is frequently modelled *in vitro* to assess its cellular effects [1]. In this study, we investigated the time-dependent effects of hypoxia on human brain endothelial cells (HBEC-5i) using Fourier Transform Infrared Spectroscopy (FTIR) and Raman Spectroscopy (RS). Cells were grown in normal oxygen levels (37°C, 5% CO_2) and low oxygen conditions (1% O_2) for 3, 6, 9, 12, and 24 hours (Figure 1). Our analysis revealed that hypoxia leads to significant alterations in cellular structures. As a result of the adaptation mechanism, we observed significant alterations in lipid composition, including elongation of acyl chains, a transient decrease in fatty acid esters, and temporary changes in free fatty acids. Global changes in protein secondary structures were observed under hypoxic conditions (Figure 1). Additionally, hypoxia caused a shift in DNA conformation from B-form to A-form. RNA structure was also impacted, as indicated by band shifts to lower wavenumbers, possibly reflecting changes in metabolic activity. These findings reveal the complex response of brain endothelial cells to oxygen deficiency and highlight the value of FTIR and Raman spectroscopy in studying adaptations relevant to neurodegenerative research.

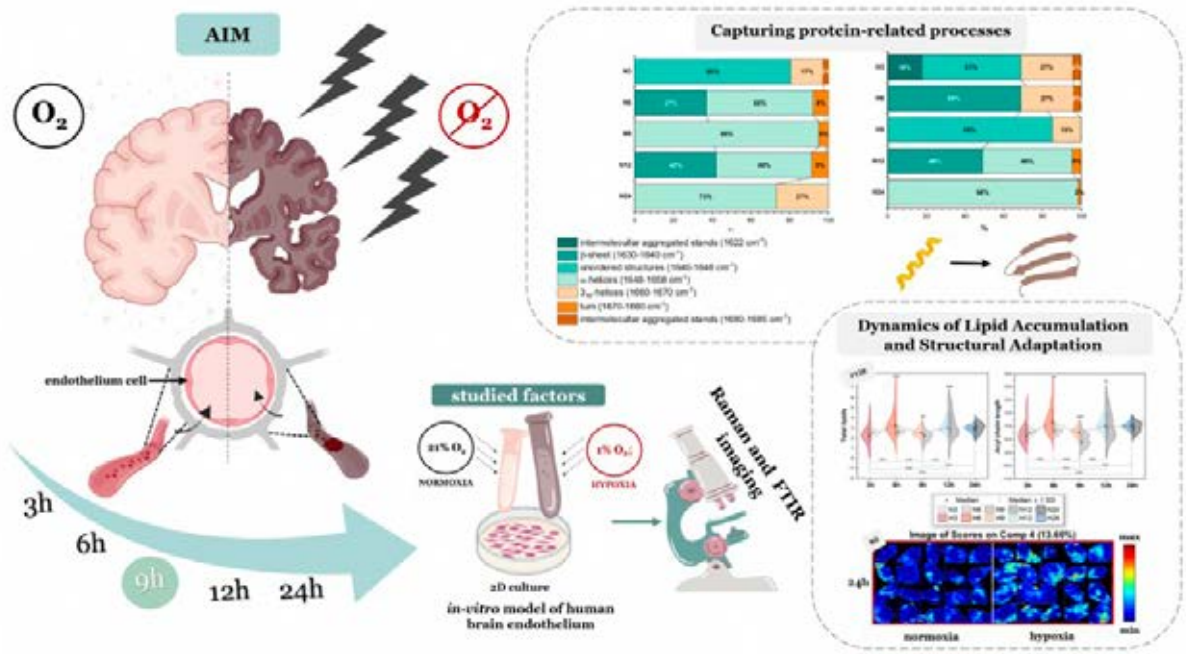
This work was supported by the Polish National Science Center (OPUS 21, grant No. 2021/41/B/ST4/02000) and a grant from the Faculty of Chemistry under the Strategic Programme Excellence Initiative at Jagiellonian University.

References:

[1] A. Pragnąca, A. Antolak, Z. J. Krysiak et al., Scientific Reports 15, 26112 (2025)

Keywords: spectroscopic imaging, chemometrics, hypoxia, brain endothelium, neurodegenerative diseases

Figure 1 Schematic overview of time-dependent hypoxia in brain endothelial cells.



[Abstract:0311] [Non-linear/Time-resolved]

Lattice Dynamics of Transparent Rock-Forming Minerals Probed by Complementary Frequency-Domain and Time-Domain Raman Spectroscopy

***Sergey G Pavlov*[1], *Yoo Kyung Ha*[2], *Emma Kinne*[2], *Iris Weber*[3], *Ralf T Schmitt*[4], *Nikola Stojanovic*[1], *Michael Gensch*[2]**

[1]*Institute of Space Research, German Aerospace Center (DLR), Berlin, Germany*
[2]*Institute of Physics and Astronomy, Technische Universität Berlin, Berlin, Germany, Institute of Space Research, German Aerospace Center (DLR), Berlin, Germany*
[3]*Institut für Planetologie, Universität Münster, Münster, Germany*
[4]*Museum für Naturkunde - Leibniz Institute for Evolution and Biodiversity Science, Berlin, Germany*

The complementary use of frequency-domain and time-domain Raman spectroscopy can be utilized as a versatile analytical tool for the in-depth characterization of crystal lattice dynamics (post-metamorphic and present) in natural minerals. While conventional frequency-domain Raman spectroscopy (FDRS) is a standard tool and highly sensitive for identifying the full spectrum of vibrational modes, time-domain Raman spectroscopy (TDRS) offers a unique ability to directly observe the coherent time-evolution of these lattice vibrations, including materials with strongly luminescent inclusions.

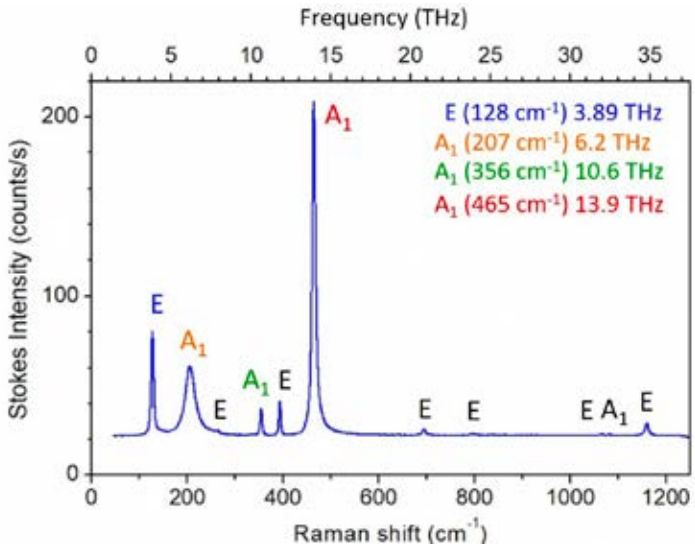
Precise determination of the vibrational frequency, spectral line shape and its dynamic counterpart are keys for accurate assignment of possible crystal metamorphisms, temperature, and/or shock-related. Fourier-transform (FT) techniques, such as continuous wave FT-Raman and TDRS, offer high precision in absolute frequency when a large time window is measured. The linewidth of a Raman peak in static spectroscopy corresponds to the phonon lifetime based on the uncertainty principle. The line broadening typical for natural minerals due to impurities, strain or defects, provides insights into the alteration of minerals, assuming it can be isolated from the line shapes corresponding to the true anharmonic phonon decay rate. TDRS directly measures the dynamics of phonon modes via the detected time-transients of transmitted, reflected or scattered fs light pulses, thereby giving direct insights into the anharmonicity of lattice vibrations and inhomogeneous broadening.

Using synthetic crystals as reference lattices, we investigated whether it is possible to disentangle homogeneous and inhomogeneous line broadening in natural minerals by a comparative analysis of frequency-domain Raman spectroscopy (dispersed static visible range Raman spectrometer) and time-domain Raman spectroscopy (ultrashort pump-probe measurement setup). The transients/spectra were collected in the overlapping range of both techniques (100-1300/cm) and stage delays (0-5 ps), and at spectral resolutions of a few 1/cm. This range allows comparison of key vibrational modes (ridging/lattice, breathing, bending, stretching) in chemically simple crystals translucent at 800 nm, chosen for this study, including silicates, carbonates and metal oxides.

In this work, we compare the FDRS line shapes with the evolution of the same modes observed in TDRS, where the decay times are obtained by fitting a cumulative sum of transients at phonon frequencies (Figs. 1,2,3).

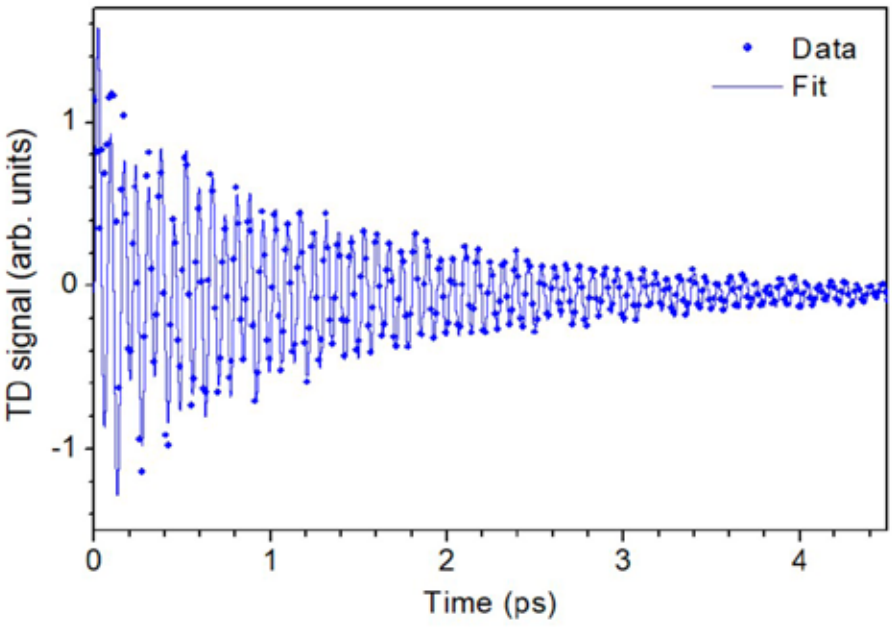
Keywords: time-resolved spectroscopy, rock forming minerals, lattice dynamics

Figure 1



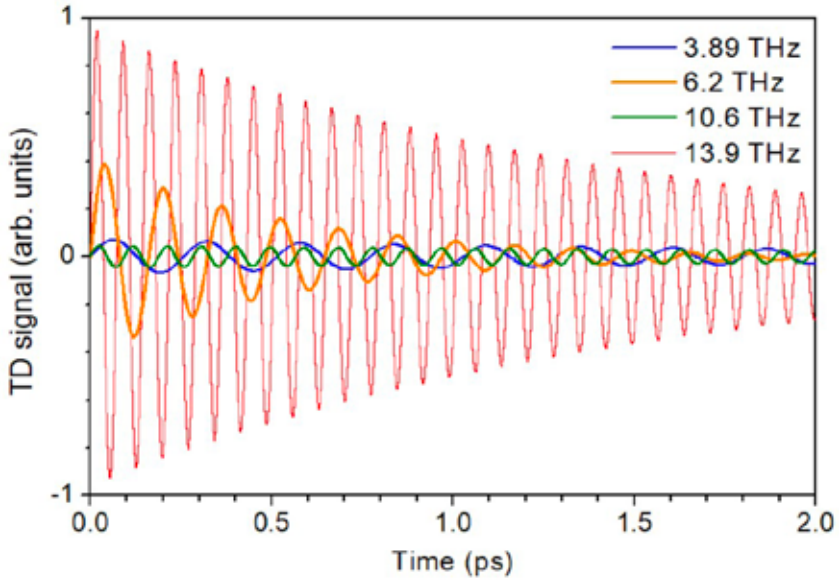
Conventional (Frequency-Domain) Raman spectrum of a z-cut crystalline synthetic quartz plate (Korth Kristalle, Germany) taken by a commercial WITEC α-300 Raman microscope under a 532 nm excitation laser, < 3 mW, backscattering geometry.

Figure 2



Time-Domain Raman measurement of the same sample taken in transmission geometry (points), and the cumulative fit (line). Pump and probe pulses had a central wavelength of 800 nm and a pulse duration of 35 fs.

Figure 3



Decaying oscillation corresponding to the evolution of the strongest phonon modes of quartz. The sum of all the oscillations is the resultant transient transmission measurement shown in Fig. 2. The derived damping constant at each phonon frequency is compared with the fitted line shape from the FDRS spectrum.

Oral Abstracts

[Abstract:0314] [Materials]

Process Control of Zeolite Synthesis Using in Line Raman Spectroscopy: A Comparison with Off Line X-Ray Difraction Analysis

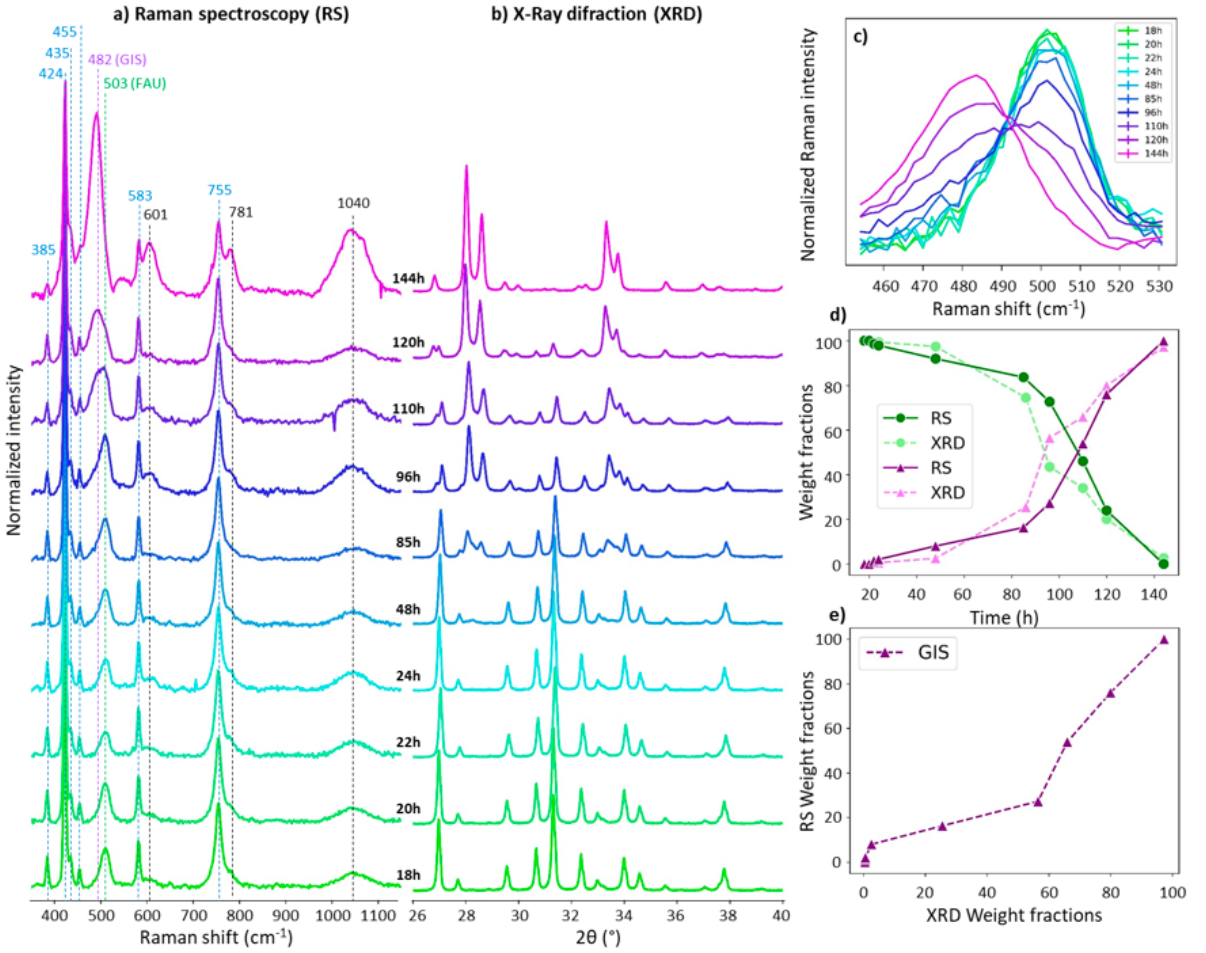
***Nicolás Coca López*[1], *Fileto Rodríguez*[2], *Frederik Tielens*[2], *Monica Calatayud*[5], *Lars Fahl Lundegaard*[3], *Xiang Li*[1], *Enrique Lozano Diz*[4], *Søren Birk Rasmussen*[3], *Miguel A. Bañares*[1], *Raquel Portela*[1], *Pablo Beato*[3]**

[1]*Instituto de Catalisis y Petroleoquimica (ICP), CSIC, Madrid, Spain*
[2]*Vrije Universiteit Brussel, Brussels, Belgium*
[3]*Topsoe A/S (HQ), DK-2800 Kongens Lyngby, Denmark*
[4]*ELODIZ Ltd., High Wycombe, UK*
[5]*Sorbonne Université, Paris, France*

Zeolites are a family of microporous crystalline materials which have an indispensable role in the chemical industry as catalysts. Zeolites can be synthetized from a simple precursor solution, following a straight forward recipe [Twu et al. Zeolites 11(7), (1991)]. However, this process is not thermodynamically stable and interzeolite conversion to undesired byproducts might occur [Mallette et al., JACS Au, 2, 10 (2022), 2295–2306]. Commercial production of metastable zeolites relies on ex-situ X-ray diffraction (XRD) for synthesis monitoring. XRD allows to quantify the fraction of different zeolite structures. However, this requires sample extraction, preparation, and analysis by qualified operators, which is inconvenient, time consuming and prevents from stopping the reaction at the optimal moment. Here we propose Raman spectroscopy as alternative, in-line, process control technology to speed up sample analysis and simultaneously probe solid and liquid phases, demonstrating its use to monitor the transformation of faujasite (FAU) into gismondine (GIS). Non-negative least squares (NNLS) algorithm was employed to track the relative abundances of FAU and GIS throughout the crystallization process using only the pure FAU and GIS Raman spectra in operational conditions as inputs. The resulting Raman derived FAU and GIS phase fractions show strong agreement with XRD based Rietveld refinements, enabling continuous tracking of crystalline phase evolution without invasive sampling. Complementary DFT based vibrational calculations provide molecular level interpretation of framework specific Raman signatures, confirming the structural origin of the main features. A preliminary multivariate regression model further demonstrates the feasibility of predicting GIS weight fractions directly from Raman spectra. Overall, the results establish Raman spectroscopy as a robust, non-destructive, and temporally resolved tool for quantifying zeolite crystallization kinetics. The methodology is directly applicable to industrial process monitoring and offers a foundation for future real time control strategies in zeolite synthesis and other crystallization driven chemical manufacturing processes.

Keywords: in situ spectroscopy, process control, crystallization monitoring, machine learning, chemometrics,

Interzeolite Conversion Monitoring



Faujasite (FAU) to gismondine (GIS) interzeolite conversion monitoring. (a) In situ Raman spectra and (b) ex situ X-ray diffractograms of zeolite slurry taken at different synthesis times. (c) Normalized Raman spectral region of interest. (e) Weight fractions over time and (e) their correlation for GIS.

[Abstract:0315] [Non-linear/Time-resolved]

Vibrational Signature of 1Bu+ and Hot 2Ag- Excited States of Carotenoids Revisited by Femtosecond Stimulated Raman Spectroscopy

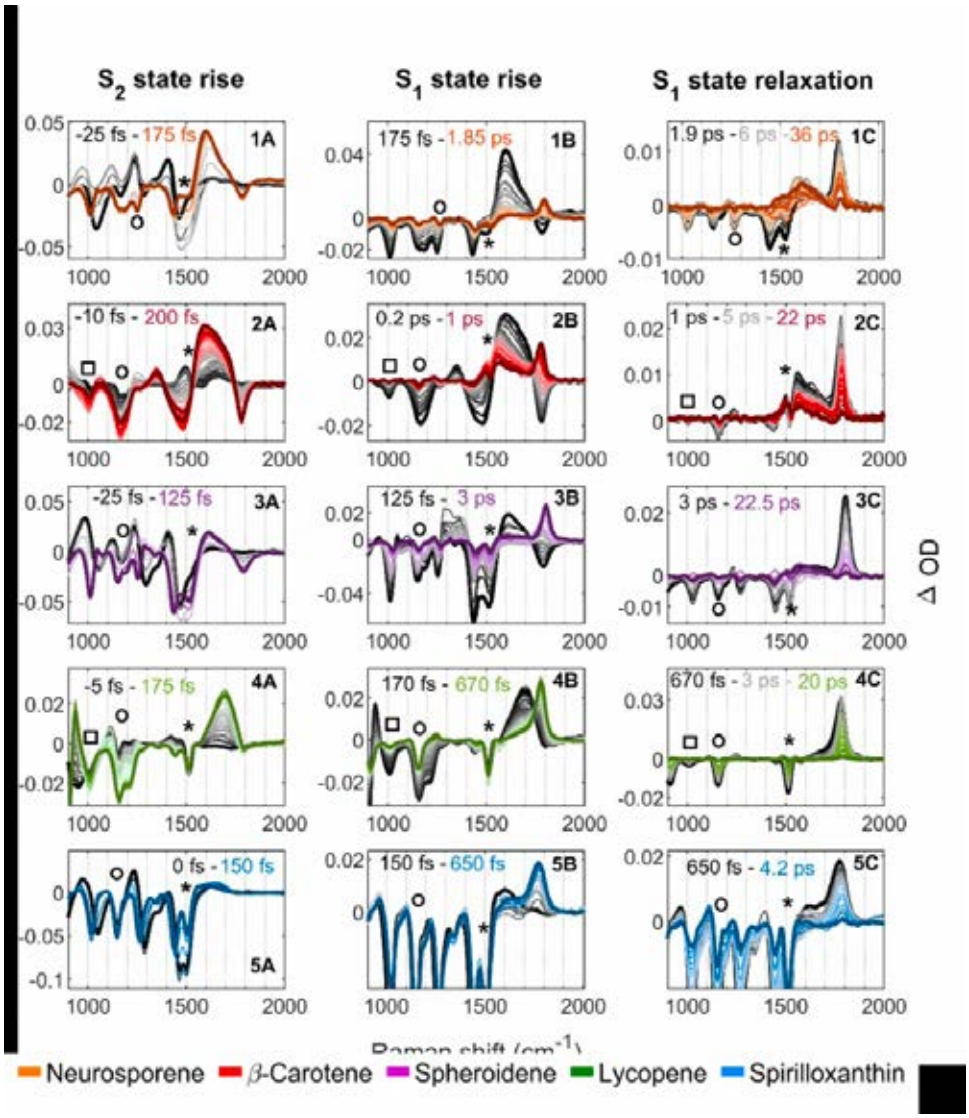
***Miroslav Kloz*[1], *Petra Čubáková*[2], *Michal Koblizek*[4], *Andrej Hovan*[3], *Alastair T. Gardiner*[4], *Tomas Polivka*[2]**

[1]*The Extreme Light Infrastructure ERIC, ELI Beamlines Facility, Za Radnicí 835, Dolní Břežany, Czech Republic*
[2]*Department of Physics, Faculty of Science, University of South Bohemia, Branišovská 1760, 370 05 České Budějovice, Czech Republic*
[3]*Department of Biophysics, Faculty of Science, P.J. Šafárik University in Košice, Jesenná 5, 041 54, Košice, Slovakia*
[4]*Laboratory of Anoxygenic Phototrophs, Institute of Microbiology, Czech Academy of Sciences, 379 81 Třeboň, Czech Republic*

The significance of carotenoids in biological systems cannot be overstated. Their functionality largely arises from unique excited-state dynamics, where photon absorption promotes the molecule to the optically allowed 1Bu+ state (conventionally S2), which rapidly decays to the optically forbidden 2Ag- state (S1). While the vibrational signature of the S1 state is well established, that of the initial S2 state has remained elusive. In this work, we identify a consistent S2-state vibrational signature across five different carotenoids and explain the challenges in isolating this signature. Resonance conditions in the near infrared region cause the S2 signal to appear as a complex superposition of contributions from stimulated emission to the ground state, excited-state absorption (S2 to Sm), and vibrationally inverted S1 signals. This results in a mix of positive and negative features that are not trivial to disentangle. After careful analysis, we isolated the genuine S2 signature, characterized by a C=C stretch near 1600 cm−1 and a C–C stretch near 1350 cm−1. The remaining signals originate from the ground or S1 states but are virtually inseparable from the FSRS signal on S2-state timescales. Our findings resolve a long-standing spectroscopic challenge and clarify the early excited-state dynamics of carotenoids.

Keywords: FSRS, carotenoids, femtosecond, Bu+, Ag-, stimulated emission

Carotenoids ultrafast signatures



Unified picture of S2/S1 relaxation observed via fs Raman spectroscopy

[Abstract:0317] [SERS/TERS/Plasmonics]

Nanoscale Chemical Imaging of Interfacial Reactions by Tip-Enhanced Raman Spectroscopy

Liqing Zheng

School of Chemistry, Nanjing University, Nanjing, China

Interfacial reactions play important roles in electrochemistry and heterogeneous catalysis. It is still challenging to investigate interfacial reactions with nanoscale spatial resolution, in a non-destructive manner. For a thorough understanding of interfacial reactions, we need an analytical tool to provide information on the surface and the molecules with high spatial resolution and high sensitivity.

Tip-enhanced Raman spectroscopy (TERS) simultaneously provides chemical fingerprint information with single-molecule sensitivity and topographic information with nanometer spatial resolution. TERS has been demonstrated to be a powerful analytical technique for the study of interfaces. It has been used to monitor different interfacial reactions, since it enables the correlation between the chemical performance and the surface structure.

We used TERS to investigate different interfacial reactions, such as on-surface photoisomerization of molecular switches, on-surface coordination, click reactions, and heterogenous catalytical reactions, etc. In this talk, we will first present the applications of TERS mapping for probing the hydrogenation reaction of nitroarene, with a spatial resolution of 10 nm. We provide a spectroscopic evidence for the hydrogen spillover from Pd to Au within a distance of 20 nm. Next, we study the plasmon-induced protodeboronation reaction on a metal surface using TERS. TERS imaging was used to monitor the plasmon catalyzed reaction under different reaction conditions. We find that the reaction activity and selectivity of the plasmon catalyzed reaction can be tuned by changing the reaction microenvironment, such as laser power, pH, and coreactants. Finally, we employ TERS imaging to study the click reaction for functionalizing monosaccharide molecules on Au surfaces. Although different monosaccharides contain similar functional groups, their TERS spectra are distinct and can be well resolved using their fingerprint, owing to the single-molecule sensitivity and ultrahigh spatial resolution of TERS. Moreover, TERS maps reveal that two different monosaccharides that were coassembled on the Au surface form nanodomains at various areas, due to comparative adsorption. With this, we conclude that TERS is a potent analytical tool for interfacial reactions, especially in heterogeneous catalysis.

Keywords: Tip-enhanced Raman spectroscopy imaging, heterogeneous catalysis, hydrogen spillover, plasmon-induced catalytic reaction, click reaction, interfacial reactions

[Abstract:0320] [Biology/Biomedicine]

Serum Raman Spectroscopy and Metabolomics Reveal Early Events in Oral Carcinogenesis

***Priyanka Arun Jadhav*[1], *Arti Hole*[1], *Ankit Halder*[3], *Sanjeeva Srivastava*[3], *Murali Krishna Chilakapati*[1]**

[1]*Advanced Centre for Treatment Research and Education in Cancer (ACTREC), Tata Memorial Centre (TMC), Sector-22, Kharghar, Navi Mumbai 410210, India*
[2]*Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400094, India*
[3]*Department of Biosciences and Bioengineering, Indian Institute of Technology Bombay, Powai, Mumbai 400076, India*

Oral cancer continues to pose a major global health challenge due to diagnosis at advanced stages of the disease. This highlights the pressing need for screening strategies that are minimally invasive, rapid, and objective to detect early events associated with cancer development. This study utilized the well-established hamster buccal pouch (HBP) model of DMBA-induced oral carcinogenesis to investigate disease progression. Weekly photographic monitoring of the HBP over a period of 14-weeks clearly documented the transition from normal mucosa to malignant stages. During which serum samples from DMBA-treated and age-matched control groups were analyzed using Raman spectroscopy (RS) and mass spectrometry (MS) to capture biochemical and metabolic alterations associated with development of oral cancer. Serum RS analysis could detect early changes, with PC-LDA scatter plots showing distinct clustering across stages (S0 to S4). Furthermore, MCR-ALS indicated significant variations in protein and lipid components as the disease progressed. MS-based PCA of control samples confirmed that the metabolic differences observed in DMBA-treated group were related to carcinogen exposure rather than age-related variations, supporting the RS findings. Metabolites, including uric acid, lysophosphatidylcholine, palmitoylcarnitine, and valine, exhibited significant alterations. These metabolites are involved in lipid metabolism, oxidative stress, and inflammatory processes that are closely associated with oral cancer progression. Thus RS-MS approach provides comprehensive insights into the development of oral carcinogenesis. Although MS provides high molecular specificity, its use is limited by high cost and complex workflows. In contrast, serum RS shows potential as an early screening tool for oral cancer, particularly in high-risk populations.

Keywords: Oral cancer progression, Raman spectroscopy, Hamster buccal pouch model, Mass spectrometry, Metabolic alterations

[Abstract:0321] [Novel Approaches]

Terahertz Raman Optical Activity as A Window into G-Quadruplex Self-Assembly

Štěpán Jílek[1], Lucia Ďuríšková[1], Martina Valášková[1], Alžbeta Bundová[1], Josef Kapitan[2], Mohammed Siddhique Para Kkadan[3], Petr Bour[3], Václav Profant[1]

[1]Institute of Physics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 121 16 Prague 2, Czech Republic
[2]Department of Optics, Faculty of Science, Palacky University Olomouc, 17. Listopadu, 771 46 Olomouc, Czech Republic
[3]Institute of Organic Chemistry and Biochemistry AS CR v.v.i., Flemingovo namesti 2, 166 10 Prague 6, Czech Republic

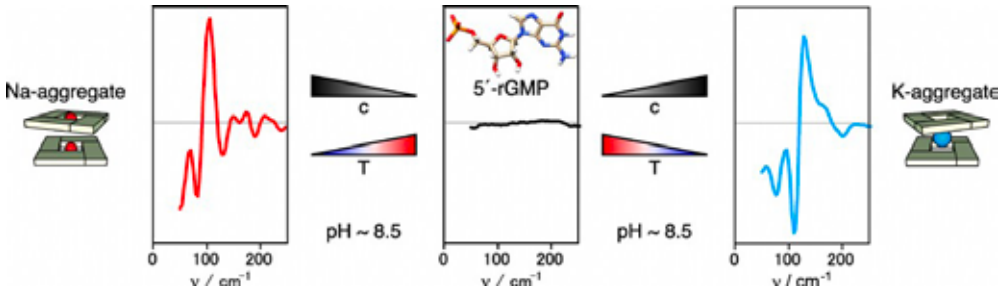
Supramolecular chirality arising from nucleic-acid self-assembly remains challenging to probe experimentally, particularly in weakly bound, structurally polymorphic aggregates. Mononucleotide G-quadruplexes (mG4) formed by guanosine monophosphate (GMP) provide an attractive model system for studying such hierarchical organization. Their formation involves stacking of G-quartets stabilized by monovalent cations, giving rise to structurally polymorphic assemblies whose detailed organization remains difficult to characterize by conventional spectroscopic methods.

Vibrational optical activity, and Raman optical activity (ROA) in particular, is uniquely sensitive to such higher-order chiral organization. Upon formation of GMP quadruplex assemblies, the ROA spectra undergo pronounced changes accompanied by the build-up of an unusually strong signal in the low-wavenumber (terahertz) region below 200 cm^{-1}. This spectral response is absent in monomeric species and reflects collective vibrational modes associated with the supramolecular arrangement of stacked G-quartets, providing a direct spectroscopic marker of quadruplex formation (Figure 1).

In this contribution, we systematically map the multidimensional landscape of GMP self-assembly using ROA combined with Raman spectroscopy, chemometric analysis, and quantum-chemical simulations. Concentration-dependent measurements resolve the transition from monomer stacking to quadruplex formation, while temperature and pH experiments define the stability limits of the assemblies, including gel formation. The influence of various monovalent cations (Li^+, Na^+, K^+, Rb^+, Cs^+, and NH_4^+) reveals pronounced structural polymorphism, while comparison of ribose- and deoxyribose-containing nucleotides highlights the key role of the 2′-hydroxyl group in stabilizing the aggregates. Quantum-chemical simulations link the terahertz ROA bands to torsional ordering between stacked G-quartets, demonstrating that low-frequency ROA provides a sensitive probe of collective modes and supramolecular chirality in nucleic-acid assemblies.

Keywords: Raman optical activity, Terahertz spectroscopy, G-quadruplex, Supramolecular chirality, Self-assembly

Figure 1



Low-wavenumber (THz) ROA spectra of 5′-rGMP self-assembly. The transition from monomer (black) to Na- (red) or K-type (blue) mG4 aggregates is promoted by increasing concentration (c) and suppressed by increasing temperature (T), as indicated by the gradient triangles.

[Abstract:0322] [Non-linear/Time-resolved]

Mapping the Vibrational States in Retinal and Retinal Schiff Base by FSRS

***Shilpa Kurupath Bhavadas*[1,2], *Petra Chrupkova*[1], *Petra Chrupkova*[2], *Cesar Bernado*[1], *Miroslav Kloz*[1]**

[1]*The Extreme Light Infrastructure (ELI) ERIC,Za Radnici 835, Dolni Brezany, Czech Republic*
[2]*Department of Biophysics, FSc, University of South Bohemia, České Budějovice, Czech Republic*

Retinal and retinal Schiff base (RSB) are fundamental polyene chromophores that mediate primary photochemical processes in vision and several light-driven biological systems. Despite extensive spectroscopic investigations, the ordering and interplay of their low-lying excited states remain not fully understood, particularly the role of dark states in mediating triplet formation.

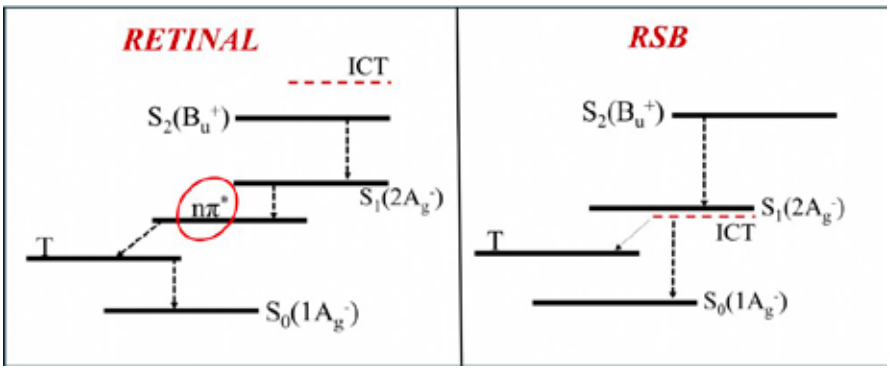
Here we investigate how subtle chemical modifications alter excited-state relaxation pathways by comparing retinal and its unprotonated Schiff base using femtosecond stimulated Raman spectroscopy (FSRS) in combination with transient absorption spectroscopy.

Our studies reveal that the presence of specific terminal groups strongly influences π-electron delocalization and bond length alternation (BLA) along the conjugated polyene chain, which in turn reshapes the excited-state landscape. In retinal, the carbonyl group introduces a low-lying nπ* state that transiently localizes electron density and reduces π-conjugation. FSRS spectra show early-time broadening in the C=C stretching region, consistent with reduced delocalization prior to triplet formation. At longer delays, characteristic triplet vibrational signatures appear, including a downshift of the C=C stretching mode and an upshift of the C–C stretching mode, reflecting redistribution of bond order in the triplet state. In contrast, retinal Schiff base lacks the carbonyl functionality, suppressing the nπ* state and promoting dynamics more analogous to long-chain carotenoids, where the excited-state evolution is governed primarily by interactions between Bu^+, Ag^-, and intramolecular charge transfer (ICT) states.

We propose a scheme depicting the energy ordering of the vibrational states in Retinal and RSB based on the evidence from FSRS and TA measurements.Our study highlight the sensitivity of polyene photophysics to local chemical structure and provide new insight into how they control excited-state dynamics in retinal-based chromophores.

Keywords: Femtoseond stimulated Raman spectroscopy,Retinal, Time resolved

Fig1. The proposed scheme



[Abstract:0324] [Biology/Biomedicine]

Raman and FTIR Imaging Sensitivity and Specificity in Decoding Cellular Transformations and Dysfunctions in 2D and 3D In Vitro Models

***Kamilla Malek*[1], *Anna Antolak*[1], *Karolina Augustyniak*[1], *Aleksandra Pragnąca*[2]**

[1]*Faculty of Chemistry, Jagiellonian University in Krakow, Gronostajowa 2, 30-387 Krakow, Poland*
[2]*Doctoral School of Exact and Natural Sciences, Jagiellonian University in Krakow, prof. S. Łojasiewicza 11, 30-348 Krakow, Poland*

Raman (RS) and FTIR spectroscopies, including their imaging modalities, are proven label-free tools for detecting cellular processes in vitro—e.g., drug and plastic uptake, stress responses—and for developing ML toolboxes for biomedical use. Proper selection of in vitro models and reference techniques is essential for validating spectroscopic findings, given cell-type variability, cell–cell interactions, and process dynamics. Although RS and IR provide complementary molecular information, data collection and fusion are demanding. Here, we summarize our IR/RS imaging methodology for probing eukaryotic cells of diverse origins and exposures [1-3].

Raman and IR maps reveal molecular signals from core biomolecules localized in organelles, but in different ways [1]. This spectroscopic "barcode" enables us to phenotype cancer cells, blood–brain barrier (BBB) cells, and progenitors in low-density 2D cultures—models with high metabolic and proliferative rates and minimal cell–cell communication—making them suited for assessing metabolic responses to stressors [2]. Using established IR/RS metrics and chemometrics (CA, MCR, PCA, PLS), we distinguish experimental groups and detect changes in primary metabolites and stress markers at single-spectrum and map scales [2]. When in vitro models involve direct cell–cell contact or tissue-like structures, the barcode persists, but hyperspectral data require deeper analysis to reveal transformations, new structures, or molecular exchanges relevant for ML prediction. We illustrate these approaches with stem cell differentiation, metastatic cancer cell migration, progenitor co-cultures, and BBB models [3].

This work was supported by the Polish National Science Center (OPUS 21, grant No. 2021/41/B/ST4/02000).

References:

[1] Anal. Chem., 2025, 97, 16374

[2] Cancers, 2021, 13, 123; Cell Mol. Life Sci., 2022, 79, 52; Inter. J. Mol. Sci., 2024, 25, 12274; Sc. Rep., 2025, 15, 26112

[3] Anal. Chem., 2026, 98, 4856; J. Lipid Res., 2024, 65, 100573; Cell Mol. Life Sci., 2023, 80, 329

Keywords: Raman and FTIR imaging, in vitro models, cell-cell interactions, spectral data mining

[Abstract:0326] [Biology/Biomedicine]

Multimodal Cardiac Tissue Analysis Using Raman Spectroscopy and AP-MALDI Mass Spectrometry Imaging in a Mouse Model of Lysosomal Storage Disease

***Elena Tolstik*[1], *Johann Dierks*[1], *Eike Ulrich Brockmann*[1], *Thomas Bocklitz*[2], *Anahi-Paula Arias-Loza*[3], *Peter Nordbeck*[3], *Sven Heiles*[4], *Kristina Lorenz*[5]**

[1]*Translational Research, Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany*
[2]*Photonic Data Science, Leibniz Institute of Photonic Technology, Jena, Germany Institute of Physical Chemistry and Abbe Center of Photonics, Jena, Germany*
[3]*Medical Clinic and Polyclinic of the University Hospital Würzburg, Würzburg, Germany*
[4]*Faculty of Chemistry, University of Duisburg-Essen, Essen, Germany & Proteomics, Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany*
[5]*Institute of Pharmacology and Toxicology, Julius-Maximilians-University Würzburg, Würzburg, Germany & Translational Research, Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany*

Early molecular changes in tissues often precede visible morphological alterations and are therefore highly relevant for early diagnosis and mechanistic understanding of pathological and genetic diseases. Conventional histology and genetic analyses often cannot resolve the localized distribution of low molecular weight compounds (<2000 Da). Raman micro-spectroscopy (RS) addresses this limitation by providing chemically specific contrast and mapping major biomolecular classes at micrometre resolution.

Here, we established a multimodal, label-free imaging approach that combines high-resolution RS (2 µm pixel size) with atmospheric pressure matrix-assisted laser desorption/ionization mass spectrometry imaging (AP-MALDI-MSI, 5 µm pixel size) on the same tissue section. RS defines the biochemical tissue landscape by mapping lipids, proteins, nucleic acids, and extracellular matrix components, while AP-MALDI-MSI identifies and spatially localizes low molecular weight compounds. We applied this approach to investigate globotriaosylceramide (Gb3) accumulation in cardiac tissue from a murine model of Fabry disease (FD), a lysosomal storage disorder caused by deficient α-galactosidase A (α-Gal A) activity. Impaired enzyme function leads to progressive Gb3 accumulation and subsequent cardiac dysfunction. Three genotypes were analyzed: wild-type controls (GLAWT), α-Gal A-deficient mice (GLAKO) modeling early or asymptomatic FD with moderate Gb3 accumulation, and transgenic G3Stg/GLAKO mice overexpressing human Gb3 synthase on a GLA-deficient background, representing symptomatic FD [Ohshima et al. 1997; Taguchi et al. 2013].

RS resolved spectral signatures of nucleic acids, proteins, collagen, and lipids, enabling spatial contextualization of structural - biochemical differences between genotypes. Complementary AP-MALDI-MSI provided molecularly specific detection and spatial mapping of Gb3 species and related lipids. To integrate both datasets, we developed an automated co-registration algorithm aligning Raman, AP-MALDI-MSI, and bright-field microscopy images from the same tissue section with 5 µm accuracy, enabling high-resolution multimodal overlays (Fig. 1) [Dierks et al., bioRxiv 2025].

Combined analysis revealed heterogeneous Gb3 accumulation patterns and distinct lipid species distributions in G3Stg/GLAKO mice compared with GLAKO and GLAWT. This hyperspectral multimodal strategy improves molecular characterization of cardiac tissue and provides new insights into disease-associated lipid heterogeneity. Importantly, the established bioanalytical pipeline enables micrometer-scale integration of RS and AP-MALDI-MSI in preclinical mouse models and offers broad potential for mechanistic studies of lipid-driven pathologies beyond FD.

Keywords: Raman Micro-Spectroscopy (RS), Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry Imaging (AP-MALDI-MSI), Multimodal Imaging Approach, Lysosomal Storage Disorder, Cardiac Tissue Analysis

Figure 1: Study design and an automated overlay of AP-MALDI-MSI and Raman images.

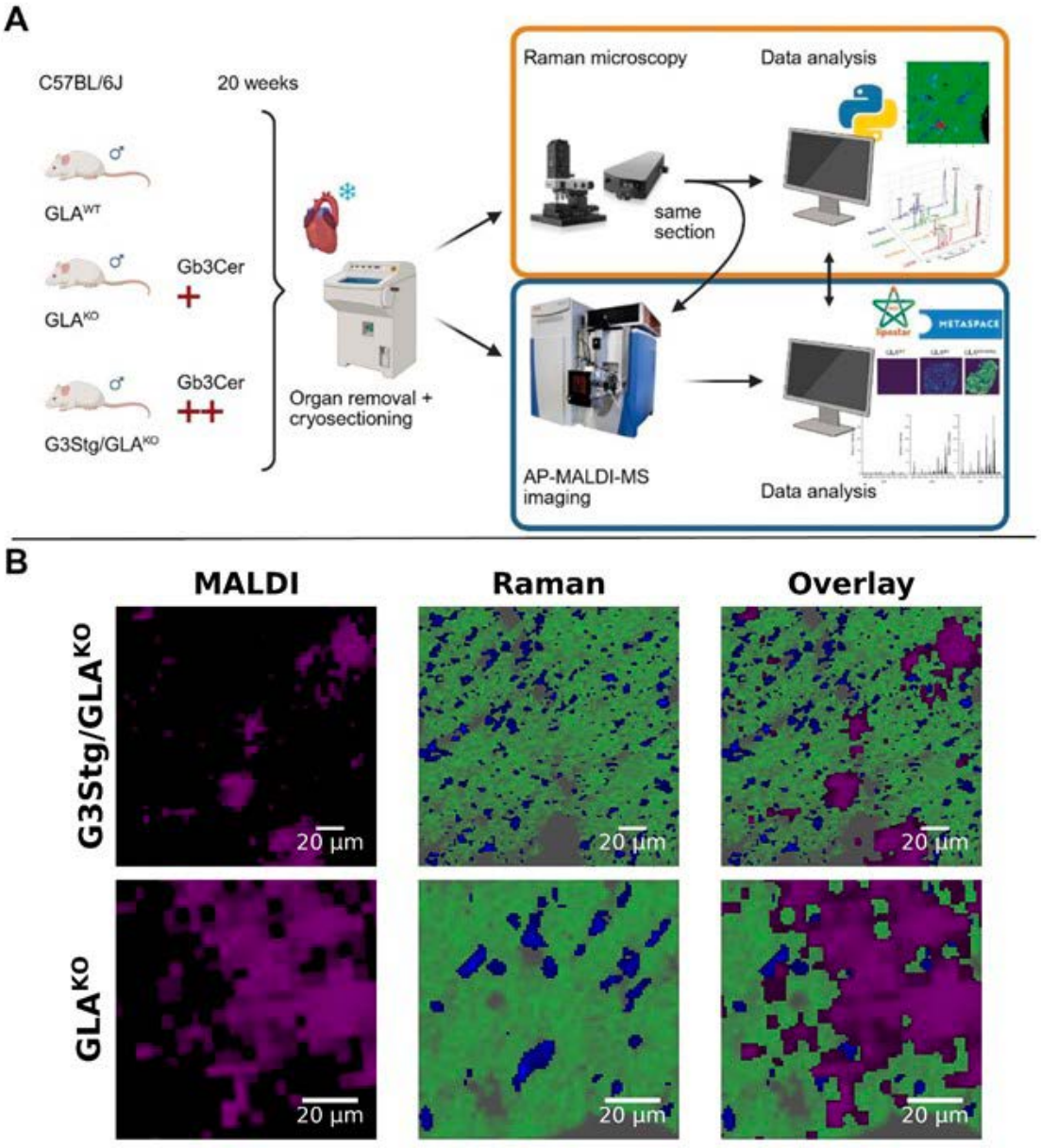


Figure 1: A) Study design. Cardiac Gb3 accumulation was analyzed in a Fabry disease (FD) mouse model comprising wild-type (GLAWT), GLA knockout (GLAKO), and G3Stg/GLAKO mice (GLA knockout with additional human Gb3 synthase expression). Heart cryosections from 20-week-old animals were examined. AP-MALDI-MSI and Raman microscopy were first performed on consecutive sections and subsequently combined on the same section (Raman imaging followed by AP-MALDI-MSI). Datasets from both strategies were integrated to increase molecular and spatial information depth. Created with BioRender.com. B) Automated overlay of AP-MALDI-MSI and Raman images. [Gb3(34:1)+Na]+ (m/z 1046.6591) accumulations (visualized in purple) from AP-MALDI-MSI overlayed with "tissue" component in green and "nucleus" component in blue derived by MCR-ALS from Raman measurements. Scale: 20 µm.

[Abstract:0328] [SERS/TERS/Plasmonics]

Moiré Tunable Raman Enhancement in Twisted MnPS3

Shilong Zhao

School of Electronic and Information Engineering, Foshan University, Foshan, China

Moiré superlattices created by interlayer twist can profoundly reshape the electronic, magnetic and optical responses of van der Waals materials, giving rise to emergent phenomena ranging from correlated insulating states and superconductivity to moiré excitons. Whether moiré reconstruction can also regulate molecular Raman enhancement, however, remains unknown. Here we show that twisted MnPS3 enhances the Raman scattering of adsorbed methylene blue, and that the enhancement is strongly dependent on twist angle. The enhancement is maximal near zero twist, decreases towards 30°, and then recovers gradually as the twist angle approaches 60°, defining a non-monotonic angular evolution over one 60° rotation cycle. This behavior suggests that the moiré superlattice modulates the interfacial charge-transfer pathway underlying Raman enhancement. Our results establish twisted MnPS3 as a moiré-tunable platform for molecular Raman amplification and provide a route to probing enhancement mechanisms in twisted two-dimensional materials.

Keywords: moiré superlattices, twisted MnPS3, surface enhanced Raman enhancement, two-dimensional materials, charge transfer

[Abstract:0331] [Biology/Biomedicine]

Label Free Assessment of Spermatozoa Status

***Maryam Jebari Ben Omar*[1], *Friedrich Striggow*[1], *Javier Plou*[2], *Yunfeng Li*[2], *Carla Solé*[3], *Mariana Medina Sánchez*[1]**

[1]*Nanobiosystems Group, CIC nanoGUNE, San Sebastián, Spain.*
[2]*Nanoengineering Group, CIC nanoGUNE, San Sebastián, Spain.*
[3]*IIS Biogipuzkoa, Paseo Dr. Beguiristain s/n, San Sebastián, Spain.*

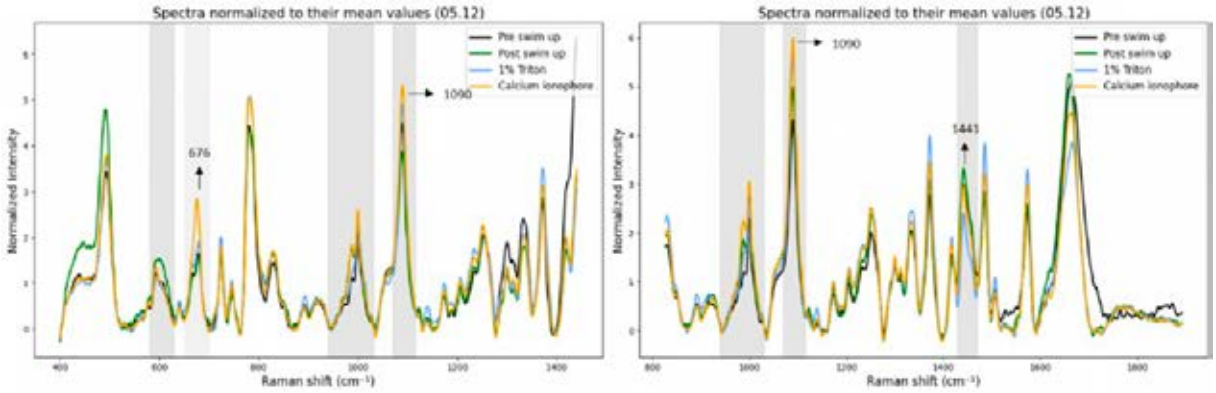
The integrity of the sperm plasma membrane and the acrosome is essential for cell survival and fertilization capacity. Most techniques for assessing sperm membrane integrity are destructive, since the sample is fixed and/or stained. Non-destructive methods, such as the Hypo-osmotic swelling test (HOST), are available, but they provide limited information. In this context, there is a need for non-destructive and non-invasive methods to assess sperm cell status. For that purpose, the use of Raman spectroscopy is being incorporated into the field of assisted reproduction. Previous Raman studies on sperm cells have mainly been performed on fixed or dried samples, which prevents the recovery of the measured cell. In contrast, the present work focuses on Raman measurements under hydrated conditions, enabling the possibility of recovering the analyzed spermatozoa after measurement.

The aim of this work is to evaluate the state of the sperm membrane through its Raman spectra. Bovine samples were measured using Raman spectroscopy under hydrated conditions (in PBS) with a 785 nm laser. Different laser powers and exposure times were tested in order to achieve the best signal-to-noise ratio without damaging the cells. In parallel, we performed flow cytometry measurements on the same samples to correlate the data with sperm viability (propidium iodide, PI) and acrosome status (peanut agglutinin-FITC, PNA-FITC). We measured samples with different treatments: before and after performing swim-up, after inducing membrane damage with 1% Triton X-100 and after inducing acrosome reaction with Calcium ionophore (Figure 1). Preliminary spectral differences were observed at Raman shifts around ~676, ~1090 and ~1441 cm-1 (Figure 1), bands commonly associated with protein and lipid components of the cell membrane, suggesting a relationship between these spectral features and sperm membrane integrity.

We present initial Raman measurements of bovine spermatozoa under hydrated conditions using a non-invasive and non-destructive approach, and correlate the spectra with the cellular state determined by flow cytometry. These preliminary results contribute to the development of a label-free method for sperm quality assessment that could allow the analysis and subsequent recovery of viable sperm cells.

Keywords: Raman spectroscopy, flow cytometry, spermatozoa, membrane integrity, acrosome

Figure 1. Mean Raman spectra from four different samples.



Mean Raman spectra from four different samples measured in two distinct spectral regions: centered at 900 cm^{-1} (left) and 1400 cm^{-1} (right) using a 1200 l/mm grating. Each spectrum represents the average of 30 sperm cells. The most relevant Raman peaks where differences between samples were observed are highlighted.

[Abstract:0332] [SERS/TERS/Plasmonics]

Rapid Manufacturing of Nanostructured Carbon-Based EC-SERS Platforms Functionalized with Gold Nanoparticles

***Angelika Łepek*[1], *Kornelia Ciurzyńska*[1], *Maciej Wróbel*[2], *Manuel Dossot*[3], *Gregoire Herzog*[3], *Mattia Pierpaoli*[2], *Jacek Ryl*[1]**

[1]*Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Gdańsk, Poland*
[2]*Faculty of Electronics Telecommunications and Informatics, Gdańsk University of Technology, Gdańsk, Poland*
[3]*LCPME, Université de Lorraine, CNRS, Nancy, France*

Rapid manufacturing approaches are increasingly employed for the development of cost-effective, fast, and customizable platforms in spectroelectrochemistry. Among these, screen-printed carbon electrodes modified with metallic nanostructures represent the most widely used systems. However, alternative architectures offering improved sensitivity, reproducibility, and structural tunability are still under active development.

In this work, we present an electrochemical surface-enhanced Raman scattering (EC-SERS) platform based on hierarchically porous laser-induced graphene (LIG) functionalized with gold nanoparticles (AuNPs). The LIG substrate provides a three-dimensional, highly conductive, and porous carbon framework, enabling efficient electron transfer and large electroactive surface area. Compared to conventional flat SERS substrates, which restrict analyte interaction to a two-dimensional interface, the developed 3D architecture enhances analyte accessibility and promotes multidirectional plasmonic interactions.

In addition, we systematically investigate various strategies for the deposition of gold nanoparticles onto the LIG surface, with particular emphasis on electrochemical methods. Special attention is given to electrodeposition via chronopotentiometry, enabling precise control over nanoparticle nucleation and growth. Based on these studies, optimal deposition parameters were identified to achieve a uniform distribution of AuNPs and maximize plasmonic activity.

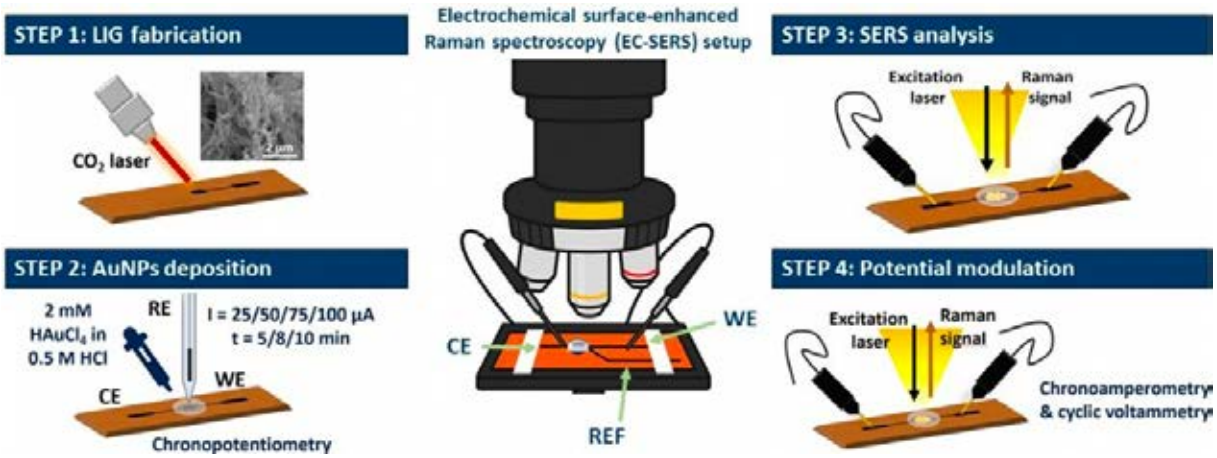
The hierarchical porosity of LIG facilitates the spatial distribution of AuNPs throughout the structure, generating a dense network of electromagnetic "hotspots." This configuration significantly increases the probability of analyte-nanoparticle interactions and enhances Raman signal intensity. Furthermore, the incorporation of AuNPs not only serves as the primary source of plasmonic enhancement but also improves the structural stability, reproducibility, and electrochemical performance of the LIG-based platform. The analytical performance of the developed EC-SERS platform was evaluated using model compounds, including Rhodamine 6G, methylene blue and 2-naphthalenethiol, demonstrating its capability for sensitive detection.

The proposed EC-SERS system demonstrates the potential of combining rapid manufacturing techniques with advanced nanostructured carbon materials for the development of next-generation sensing platforms. The integration of 3D porous graphene architectures with plasmonic nanostructures offers a promising route toward highly sensitive, reproducible, and scalable spectroelectrochemical devices.

Keywords: laser-induced graphene, EC-SERS, gold nanoparticles

Oral Abstracts

Conceptual scheme of the porous carbon-based EC-SERS platform: fabrication, functionalization, and sensing mechanism



[Abstract:0333] [Non-linear/Time-resolved]

From Molecular Vibrations to Cellular Dynamics: Real-Time Raman Study of Fatty Acid Uptake

***Anna Maria Nowakowska*[1], Aleksandra Borek-Dorosz[1], Patrycja Dawiec[1], Kenta Temma[2], Heqi Xi[2], Itsuki Yamamoto[2], Krzysztof Brzozowski[1], Joanna Profic Paczkowska[1], Hugh James Byrne[3], Kacper Siąkała[1], Katsumasa Fujita[3], Malgorzata Baranska[1]**

[1]*Jagiellonian University in Krakow, Krakow, Poland*
[2]*The University of Osaka, Osaka, Japan*
[3]*Physical to Life Sciences Research Hub, FOCAS, TU Dublin, Dublin, Ireland*

Real-time monitoring of cellular processes at the subcellular scale is essential for understanding the dynamic biochemical processes underlying cellular function and the development of pathology. Despite significant progress, the quantitative characterization of intracellular metabolic transformations remains challenging. In our studies, we combined Raman spectroscopy (RS) and stimulated Raman scattering (SRS) to bridge single-molecule sensitivity with cellular-level analysis of fatty acid uptake and lipid metabolism. The goal of the study was to analyze the kinetics of fatty acid (FA) uptake analytically over an extended temporal range from minutes to several hours.

Using the human leukemia cell line HL-60 as a model system, we investigated the uptake kinetics of deuterated palmitic acid (dPA), a well-established probe for *de novo lipogenesis*. Measurements of dPA uptake in live HL-60 cells were performed using a custom-built slit-scanning Raman microscope and two independently developed SRS systems. Data analysis was performed using various chemometric methods, including Cluster Analysis, Principal Component Analysis, and Multivariate Curve Resolution-Alternating Least Squares.

Using SRS, we visualized how dPA enters the cell during the first minutes and how its distribution changes over time in the entire cell volume. In parallel, RS provided detailed spectral information that allowed discrimination of distinct metabolic stages. We observed an initial rapid incorporation of dPA into pre-existing lipid droplets (LDs), followed by the formation of newly generated LDs exhibiting partial unsaturation, indicative of cytochrome-associated metabolic activity. The use of chemometric methods also enabled the characterization of intrinsic heterogeneity in lipid metabolism at both cellular and subcellular levels.

In our studies, we established a comprehensive framework for investigating FA uptake and processing in living cells. Our results demonstrate that real-time tracking with isotopic labeling provides valuable insights into dynamic metabolic pathways and their variability, offering new opportunities for studying lipid-related processes in health and disease, as well as for cell phenotyping.

Acknowledgments: This work was partially supported by the Foundation for Polish Science co-financed by the European Union under the European Regional Development Fund (POIR.04.04.00-00-16ED/18-00), by the National Science Center Poland, Miniatura (2023/07/X/ST4/01573) to AMN and OPUS (2024/53/B/ST4/02698) to MB, and by Jagiellonian University to AMN.

Keywords: deuterated palmitic acid, Raman spectroscopy, real-time tracking of metabolism, kinetic analysis of uptake, 3D spectroscopic imaging

[Abstract:0334] [Materials]

Comparing Smoothing Methods for Noise Reduction in Raman Spectroscopy: Impact on Plastics Identification

***Alicia Gómez López*, Raquel Portela, Nicolás Coca López**

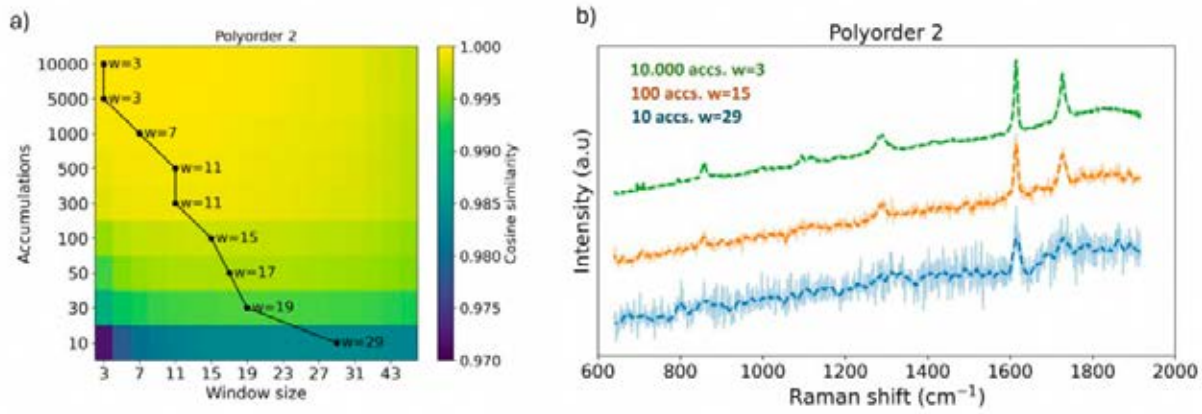
Instituto de Catálisis y Petroleoquimica (ICP), CSIC, C/Marie Curie 2, Madrid, 28049, Spain

Raman spectroscopy is widely used in microplastics research, but its performance is strongly affected by the signal-to-noise ratio (SNR) of the spectra [Coca-Lopez et al. ACS Nano 2025, 19, 38189–38218]. An increasing number of accumulations gradually reduces the noise, but it also increases measurement time and may be impractical for large screening campaigns. In this study, we explore whether optimized smoothing techniques can serve as an alternative to longer acquisition times for noise suppression while preserving relevant band shapes and intensities, thus enabling reliable data interpretation even from plastic spectra with very low SNR. We compare several denoising algorithms commonly used in spectroscopy, including moving average, moving median, Savitzky–Golay, and Whittaker–Eilers [Appl. Spectrosc. 2022, 76, 1021–1041]. First, we performed a systematic evaluation to identify the effect on the performance of key parameters, such as window size, polynomial order, or regularization strength. The optimal parameter values were estimated using different similarity metrics between smoothed, initially low-SNR plastic Raman spectra and high-SNR data obtained by accumulating a high number of spectra (Figure 1). Then, we trained a machine learning model for polymer classification using either the raw or the smoothed spectra to determine how spectra denoising and accumulating translate into better classification. This comparison supports microplastics research by providing faster and optimized polymer identification. A similar approach can also be applied wherever fast and reliable spectral analysis is required.

Acknowledgements: The authors acknowledge support from the M-ERA.NET project SURPHACE (PCI2025-163260), and the Spanish AEI project FEROX (PID2023-148983OB-100).

Keywords: signal-to-noise ratio, denoising, microplastics, similarity metrics.

Figure 1. Savitzky-Golay smoothing.



a) Window size (w) optimization using the cosine similarity metric between smoothed spectra and a reference non-smoothed spectrum obtained with 10,000 accumulations; b) Comparison between the smoothed and the raw spectra for 10 and 100 accumulations compared to the reference.

[Abstract:0335] [Non-linear/Time-resolved]

Compact, Single-Frequency High Repetition Rate Picosecond Laser for Time-Resolved Raman Spectroscopy

***Antti Penttinen*, Antti Härkönen, Mircea Guina**

Picophotonics Oy, Tampere, FINLAND

A large number of potential applications in Raman spectroscopy suffer from the so-called fluorescence problem, where overwhelming fluorescent light from the studied material prevents or hinders the detection of much weaker Raman signal. In many cases, the fluorescence problem can be significantly reduced by time-gated Raman detection, where both excitation and detection are carried out in a very short time window, prior to the occurrence of the fluorescence. As many fluorescent processes take place in nanosecond or sub-ns time scale, the excitation and detection should be done preferably in <300 ps time window.

An optimal light source for such application would need to have a stable, narrow, single-frequency spectrum, a pulse repetition rate matching the detection system, and sufficient pulse energy to create a detectable Raman signal. Optimally, the excitation source should be also small and low cost. Most picosecond laser sources however, are mode-locked lasers with wide spectrum, MHz-to-GHz repetition rate and low pulse energy and combining the optical specifications comes with a high cost.

Here, we present a compact, single-frequency picosecond microchip laser platform for time-resolved Raman spectroscopy. Laser consists of monolithic microchip laser and single-pass second harmonic generation (SHG) with 150 ps pulse duration, 150 kHz tunable pulse repetition rate and > 15 mW of average power at 532 nm. The laser features a mode-hop free spectrum with typical FWHM of < 0.06 nm and compact footprint of only 135x60x60 mm, including driver electronics, enabling portable applications. Laser suitability for the application has been demonstrated by time-gated measurement of sesame oil Raman spectrum.

In summary, we demonstrate a compact, cost-effective microchip laser platform targeted for portable time-resolved Raman spectroscopy. The key output parameters include 150 ps pulse-width, single-frequency spectrum ($\Delta\lambda$<0.06nm), 150 kHz repetition-rate and >1 kW peak power, making an excellent match for the needs of time-gated Raman spectroscopy. The presentation discusses the key technical and performance aspects with further miniaturization aiming at a credit card size footprint.

Keywords: Single-frequency laser, Time-gated Raman spectroscopy, Microchip laser, picosecond laser

Picosecond microchip laser structure

Picosecond laser structure consisting of microchip laser and single-pass second-harmonic generation.

SP05 laser source

Compact 532 nm picosecond laser source with 150 ps, 150 kHz and > 1 kW peak power.

Time-gated Raman spectrum of sesame oil measured using the compact Picophotonics laser

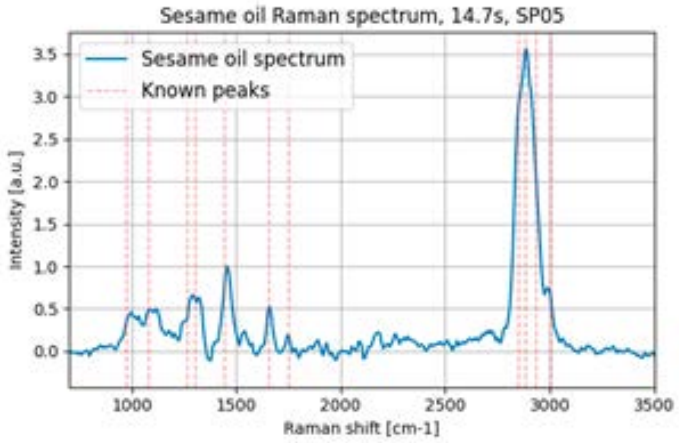


Image courtesy of RWTH Aachen, Photom project team, Merlin Schaufel

Oral Abstracts

[Abstract:0340] [SERS/TERS/Plasmonics]

Towards SERS-Based Sensing Platforms for Therapeutic Drug Monitoring in Complex Biofluids

***Aradhana Dwivedi*, Vladimir Sivakov, Juergen Popp, Dana Cialla May**

Leibniz Institute of Photonic Technology, Member of Leibniz Health Technologies, Member of the Leibniz Centre for Photonics in Infection Research (LPI), Jena, Germany, Institute of Physical Chemistry (IPC) and Abbe Center of Photonics (ACP), Friedrich Schiller University Jena, Member of the Leibniz Centre for Photonics in Infection Research (LPI), Jena, Germany

Therapeutic drug monitoring (TDM) can significantly improve the patient care, but current methods are slow, expensive and labour-intensive. This is particularly critical in sepsis and severe infectious diseases, where timely dose adjustment can directly influence treatment outcome. The reliability of surface-enhanced Raman spectroscopy (SERS) in medical diagnostics is often compromised by substrate instability, limited reproducibility, and strong matrix interference. This is especially true when working with complex biological samples such as blood. Here, we present a silver dendrite (AgD) SERS platform designed to address these challenges and advance clinically relevant drug monitoring [1]. Sulfate acts as a growth agent and passivates the surface, simplifying the fabrication process and improving shelf life. High crystallinity and sulfate passivation were confirmed by SEM, TEM, XRD and XPS analyses. The resulting AgDs can detect 4-mercaptobenzoic acid (4-MBA) at sub-femtomolar concentrations and retain consistent SERS activity for over seven months. Building on this, the AgDs were applied to clinically relevant drugs, including 6-thioguanine, methotrexate, erlotinib, doxorubicin, and moxifloxacin, with detection limits down to the sub-nanomolar range. To simulate clinically relevant conditions, these drugs were spiked into human plasma from healthy donors. Despite the complexity and interference of the plasma matrix, the drugs were detected within the required therapeutic concentration ranges. Further improvement of the detection limit was achieved through sample pretreatment, particularly protein precipitation, which reduced the complex plasma background [2]. Ongoing work is extending this platform to include the monitoring of antibiotics relevant to the management of infectious diseases, combined with machine learning analysis to improve decision-making. Together, these studies establish a practical route towards a stable, sensitive and clinically relevant SERS platform for TDM.

Acknowledgement: The Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) supported this work under grant 465289819.

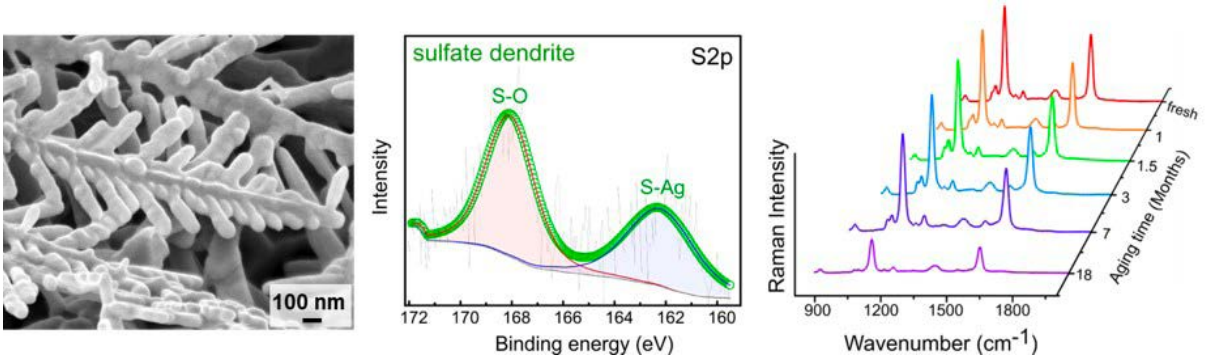
References:

[1] Dwivedi, Aradhana, et al. Advanced Science (2026): e17092.

[2] Dwivedi, Aradhana, et al. Chemosensors (2024); 12.10, 213.

Keywords: Surface-Enhanced Raman Spectroscopy (SERS), Therapeutic Drug Monitoring (TDM), Infectious Diseases, Complex Biofluids, Point-Of-Care Testing (POCT), Antibiotic Drugs

Figure 1.



SEM image of single dendrite branch, High-resolution S2p XPS spectra confirming sulfate passivation, and SERS performance over 18 months with 4-MBA.

[Abstract:0341] [Novel Approaches]

Full Vibrational Spectroscopy for Simultaneous Mechanical, Structural and Chemical Analysis

***Morteza Behrouzitabar*[1], *Kārlis Bērziņš*[3], *Renzo Vanna*[4], *Victor Alcolea Rodriguez*[5], *Ben J. Boyd*[6], *Laura D'alfonso*[1], *Cristian Manzoni*[4], *Dario Polli*[5], *Giulio Cerullo*[5], *Giuseppe Antonacci*[2]**

[1]*Department of Physics, University of Milano-Bicocca, Milan, Italy*
[2]*Specto Photonics, Milan, Italy*
[3]*Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark*
[4]*CNR-Istituto di Fotonica e Nanotecnologie (CNR-IFN), Milan, Italy*
[5]*Department of Physics, Politecnico di Milano, Milan, Italy*
[6]*Drug Delivery, Disposition and Dynamics, Monash Institute of Pharmaceutical Sciences, VIC, Australia*

Comprehensive characterization of matter across mechanical, structural, and chemical domains is essential in applications ranging from pharmaceutical manufacturing to life and materials sciences. Conventional vibrational spectroscopy techniques are typically limited to specific spectral windows, restricting the amount of correlated physical information that can be extracted from a single measurement. Here, we present an all-optical, non-destructive, and label-free method capable of acquiring the full vibrational spectrum of matter, spanning from the Brillouin and ultra-low-frequency Raman (ULFR) regimes to conventional Raman frequencies (0.1 cm^{-1} - 3,500 cm^{-1}). A birefringence-induced phase delay (BIPD) filter [Nat. Commun. 2024, 15, 1, 5202] with an optimized free spectral range provides high suppression (~60 dB) of the elastic background light and enables the simultaneous acquisition of Brillouin, ULFR, and Raman spectra from the same illumination voxel.

The application potential of this approach is demonstrated through the analysis of solid-state active pharmaceutical ingredients (APIs), where reliable differentiation of crystalline and amorphous forms is crucial for controlling solubility, bioavailability, and manufacturability. Simultaneous access to mechanical (Brillouin), structural (ULFR), and chemical (Raman) information provides a multidimensional spectral fingerprint that significantly enhances sensitivity and selectivity compared to the individual techniques. Full-vibrational spectroscopy enables discrimination between amorphous phases of APIs prepared under different conditions (Figure 1). Studies on indomethacin and indomethacin–PVP blends further demonstrate that Brillouin spectroscopy offers increased sensitivity for mixture differentiation at higher mixture concentrations, complementing Raman and ULFR analyses.

Beyond single point spectroscopy, the system is extended to full-vibrational imaging (Figure 2). Full-spectral mapping of pharmaceutical tablets enables accurate microscale identification of APIs and excipients while simultaneously revealing their mechanical and structural heterogeneity. This approach opens new opportunities for real-time, quantitative characterization and quality control in pharmaceutical manufacturing, with broader potential in life sciences and materials research through fully optical, label-free, three-dimensional multimodal imaging.

Keywords: Spectroscopy, Microscopy, Brillouin, Raman THz, Raman, API

Figure 1

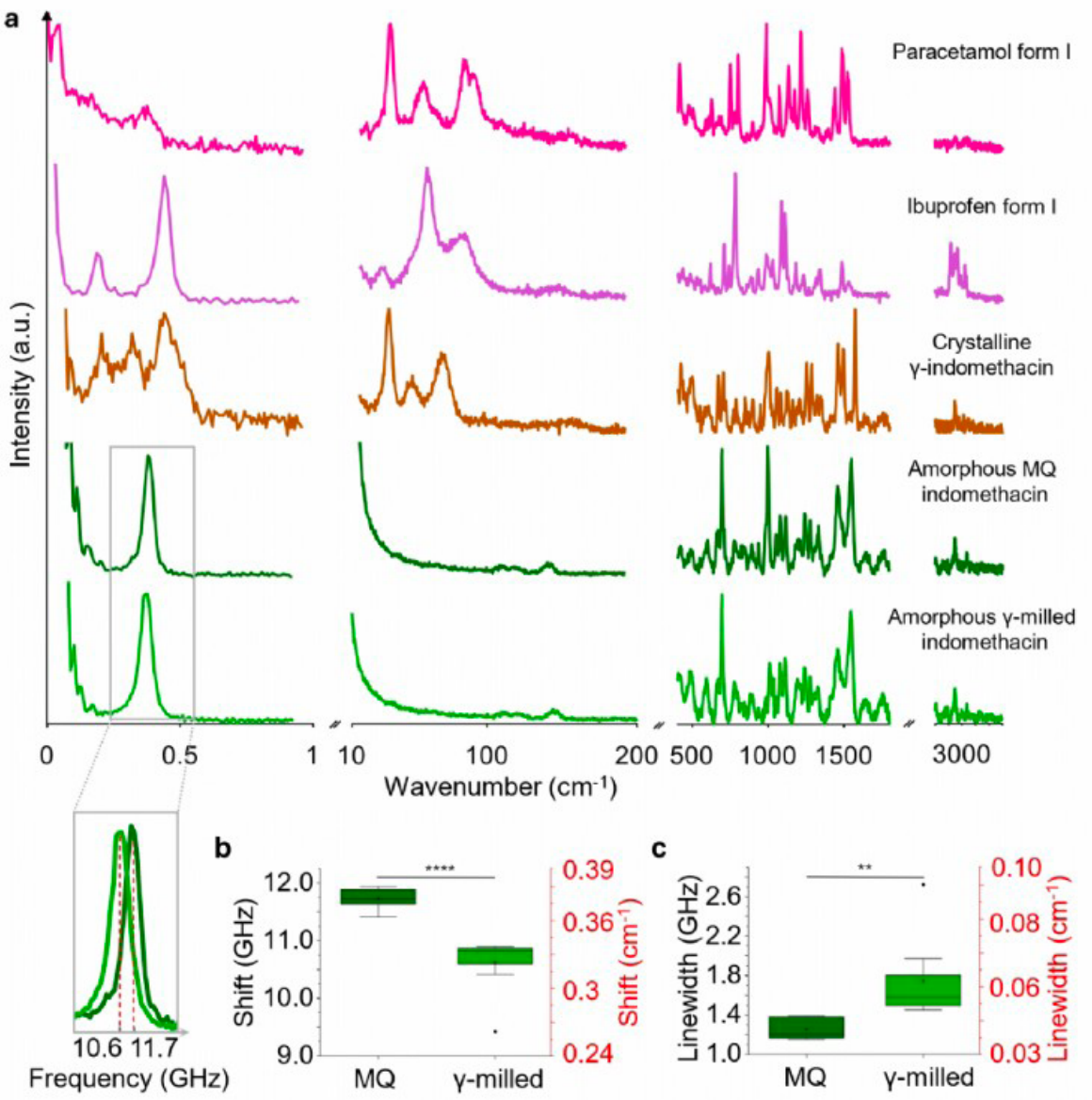


Figure 1: **Full vibrational spectral analysis of APIs reveals amorphous sample history differentiation.** **a** Full vibrational spectrum of reference APIs. Paracetamol form I, ibuprofen form I, crystalline γ-indomethacin and amorphous γ-milled indomethacin exhibit remarkably different spectral signatures across all the three different spectral domains. Amorphous melt-quenched (MQ) and γ-milled indometahcin samples show similar features in the ULFR and Raman domains while their respective Brillouin spectra manifest clear differences. **b** Indeed, a significantly higher (****$p < 0.0001$; $n \geq 5$) Brillouin frequency shift was measured for the amorphous MQ indomethacin (11.73 ± 0.12 GHz) with respect to the amorphous γ-milled indomethacin (10.60 ± 0.51 GHz). **c** On the other hand, the Brillouin peak linewidth exhibited a significantly higher (**$p < 0.01$; $n \geq 5$) linewidth for the amorphous γ-milled indomethacin (1.74 ± 0.43 GHz) with respect to the amorphous MQ indomethacin (1.25 ± 0.10 GHz).

Figure 2

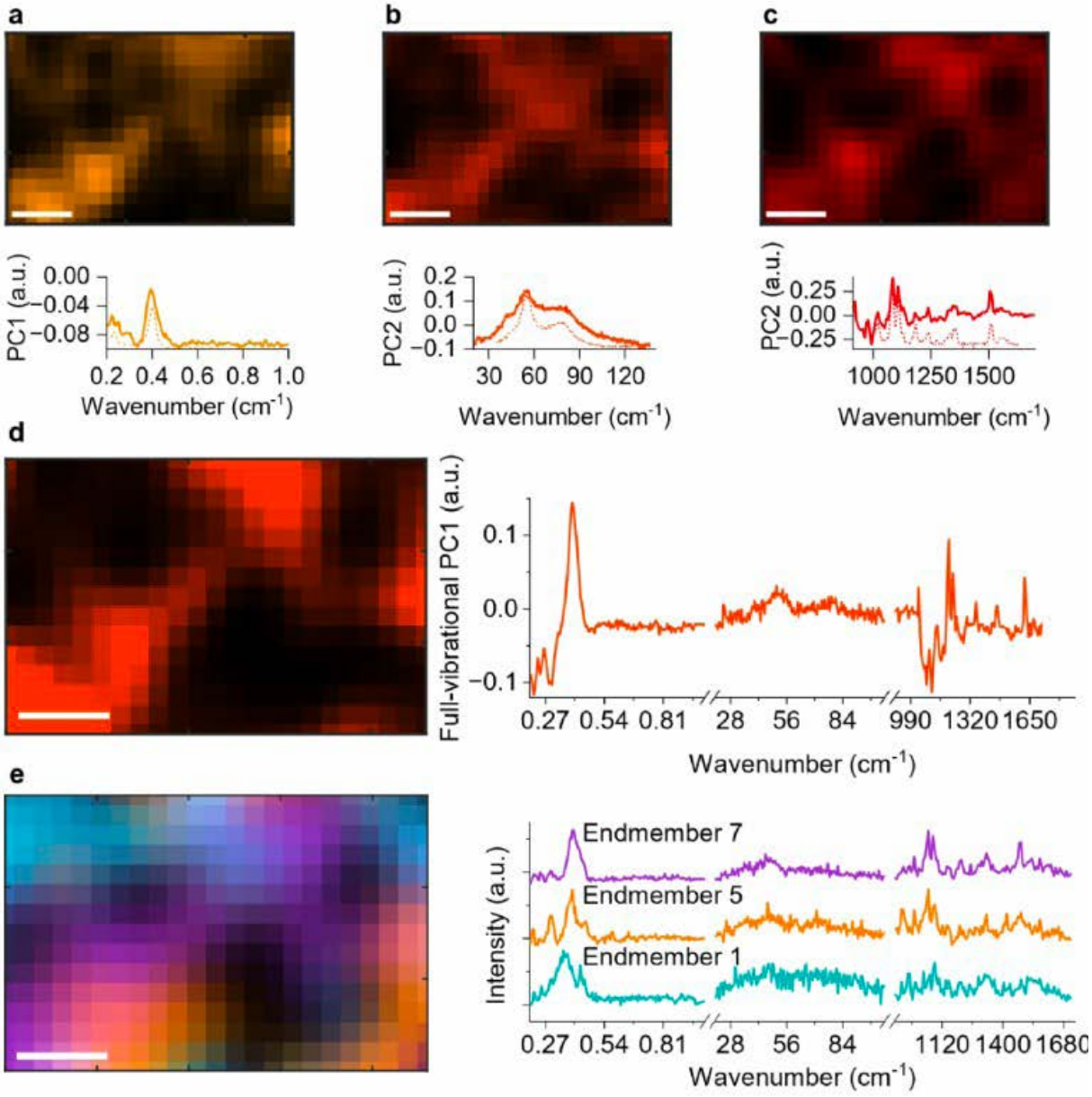


Figure 2: **Full-vibrational spectral maps of an ibuprofen tablet. a–c** Brillouin, ULFR, and Raman maps with respective loading plots associated with the relevant principal component (PC) show the mechanical, structural and chemical distribution of ibuprofen across the same field of view of a reference tablet. Dashed lines represent measured spectral data of Ibuprofen. **d** Concatenated full vibrational spectrum analyzed with PCA exhibits spectral features through the entire domain, further enhancing the image contrast and compound specificity. **e** Endmembers identified using the N-FINDR algorithm revealed mechanical heterogeneities of ibuprofen across chemically homogeneous areas. Scale bar corresponds to 100 µm.

[Abstract:0342] [Novel Approaches]

Identification and Quantification of Nanoplastics Using Raman Spectroscopy Optimised by Dielectrophoretic Pre-Concentration

***Anna Lisa Gilioli*[1], *Marta Fadda*[2], *Alessio Sacco*[2], *Korinna Altmann*[3], *Dmitri Ciornii*[3], *Frank Milczewski*[3], *Miguel Bañares*[4], *Raquel Portela*[4], *Alberto Ballesio*[5], *Andrea Mario Giovannozzi*[2], *Ettore Vittone*[1], *Andrea Mario Rossi*[2]**

[1]*University of Turin, Turin, Italy*
[2]*Istituto Nazionale di Ricerca Metrologica (INRiM), Turin, Italy*
[3]*Bundesanstalt Für Materialforschung Und-Prüfung (BAM), Berlin, Germany*
[4]*Consejo Superior de Investigaciones Científicas-Institute of Catalysis and Petrochemistry (CSIC-ICP), Madrid, Spain*
[5]*DISAT – Politecnico di Torino, Turin, Italy*

The analysis of microplastics and nanoplastics represents an emerging challenge for human health and environmental safety due to their dimensional, chemical and morphological heterogeneity. Recent European regulations (EU Regulation 2023/2055 and EU Directive 2020/2184) highlight the urgency of developing reliable analytical approaches for the study of these emerging contaminants. However, to date, there is a lack of standardised and sufficiently sensitive analytical methodologies for the chemical-physical characterisation of nanoplastics, particularly in aqueous matrices.

This work proposes a strategy for concentrating and identifying nanoplastics without complex sample preparation, combining dielectrophoresis (DEP) and Raman spectroscopy. DEP enables polymer particles to be trapped and concentrated using non-uniform electric fields generated by electrodes, whose geometry influences the trapping efficiency. Raman analysis allows the identification of chemical species and mass concentration of particles, as well as the study of their surface effects (such as oxidation) and nanoscale phenomena. The main challenge is to obtain sufficiently intense Raman spectra even at low concentrations of nanoplastics, a goal that can be achieved through dielectrophoretic trapping (Figure 1).

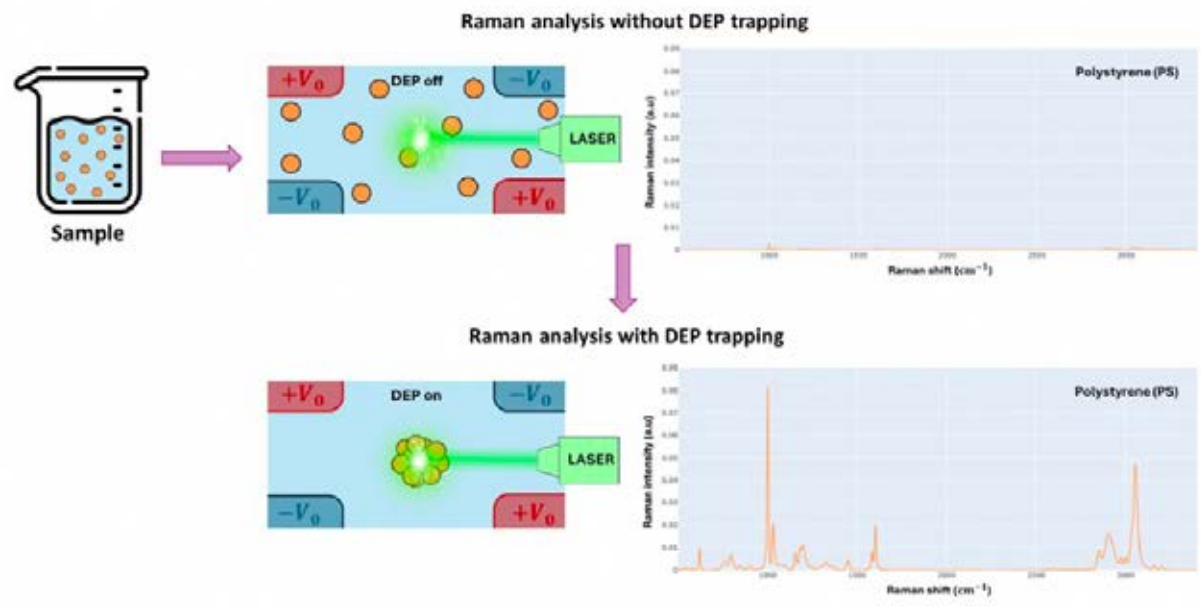
The method developed consists of four main stages: preparation of nanoplastic samples dispersed in deionised water at various concentrations; confinement of the particles using a DEP cell with quadrupole electrodes; Raman spectroscopic analysis of the confined particles; and final application of the method to a real sample of drinking water. This approach enables the rapid identification of nanoparticles with different sizes and polymeric compositions. Certified reference polystyrene spheres (60-800 nm) and polydisperse nanoplastics more representative of real samples were analysed, highlighting surface phenomena and effects associated with the small particle size.

Currently, the geometry and characteristics of the electrodes are being optimised using numerical simulations in order to improve preconcentration efficiency. The optimised configuration was then implemented and used for analysis, allowing the limits of detection (LOD) and quantification (LOQ) of the method to be determined; for certified 200 nm polystyrene nanoparticles, these values are LOD = 0.44 μg/mL and LOQ = 1.33 μg/mL, respectively.

The results demonstrate that the Raman-DEP approach can be successfully used for the physicochemical characterisation and quantitative analysis of nanoplastics in aqueous samples.

Keywords: Raman spectroscopy, Dielectrophoresis, Nanoplastics, Numerical simulation.

Figure 1



Raman analysis with or without DEP trapping

[Abstract:0344] [SERS/TERS/Plasmonics]

Active SERS Platforms: Light-Driven Micromotors and Living Algae

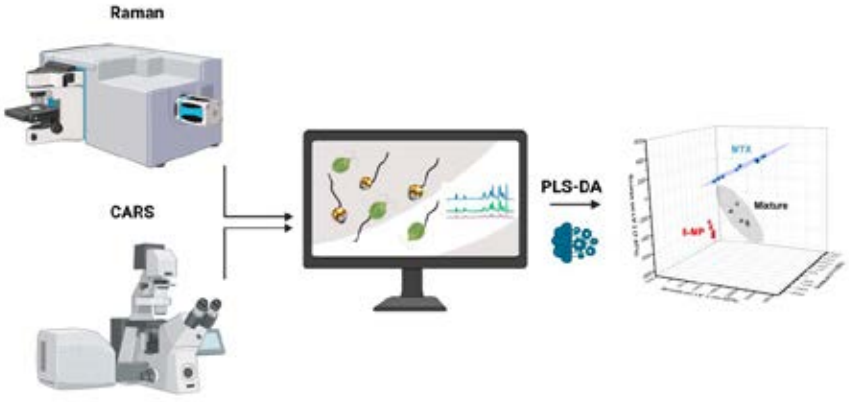
Gohar Soufi, Tijana Maric, Ziqiao Li, Casper Nisula, Zhongyang Zhang, Anja Boisen

Department of Health Technology, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

Mobile particles/microorganisms that can also function as Surface-enhanced Raman scattering (SERS) substrates have the potential to sample a larger liquid volume and preconcentrate analytes. It can also be a tool to minimize unspecific binding. We are exploring light-driven micromotors and living algae. Janus Zn/Au micromotors (MMs) are fabricated by sputtering Au onto one hemisphere of Zn microparticles, forming light-responsive spherical structures with combined photothermal propulsion and SERS sensing capabilities. The Zn/Au MMs exhibit efficient propulsion under near-infrared light, with motion driven through thermophoretic effects induced by local heating of the Au surface. CARS microscopy activates the MMs, enabling label-free, real-time tracking at 16.17 ± 2.76 μm s^{-1}. The Zn/Au MMs function effectively as active SERS platforms for single and multiplex detection of methotrexate (MTX), 6-mercaptopurine (6-MP), and their mixture with 95.5% overall predictive accuracy. When activating the MMs, the sensitivity for low concentrations of MTX showed an average of 50% enhancement. Moreover, for 6-MP which shows high affinity to gold due to the thiol group, active MMs showed prevention of affinity-driven signal plateauing result in extending the linear range. In algae, secreted reductants and biomineralization processes can generate metallic nanoparticles and plasmonic-like interfaces. The algae, by itself, is producing gold nanoparticles, is moving with directionality, and is simultaneously taking up analytes – like a scavenger. Preliminary data on the algae Chlamydomonas Reinhardtii with gold nanoparticle generation show a 55-fold increase in the Raman signal of 1,2-bis(4-pyridyl)ethylene (C = 5 mmol), which demonstrates their ability as SERS substrates. Additionally, the algae show clear clustering of gold nanoparticles (d = 12.712 ± 2.014 nm), as confirmed by TEM and EDX. The natural mobility of these live microorganisms and their directivity enable sampling specific locations within the solution containing the analyte. We have combined our active substrates with realtime tracking of individual SERS-active particles (particletracking microscopy integrated with Raman readout), enabling dynamic correlation of particle position, local environment, and spectral changes for more accurate, timeresolved sensing. New active SERS substrates enable responsive and self-accumulating sensing platforms for environmental, diagnostic, and food applications. Challenges in reproducibility, reliability, stability, and device integration remain.

Keywords: Active SERS, light-driven micromotors, Algae

Graphical abstract



[Abstract:0345] [Novel Approaches]

Toward Single-Particle Raman Microscopy of Vitrified Biological Samples at Liquid Helium Temperature

***Polina Kasyanova*, Hisham Mazal, Vahid Sandoghdar**

Max Planck Institute for the Science of Light, 91058 Erlangen, Germany

Raman imaging is highly attractive for biological research because it provides rich molecular information in a label-free manner. However, due to its intrinsically small scattering cross section, the signal-to-noise ratio in Raman measurements is severely limited. Consequently, biological samples often require illumination at high laser powers or long acquisition times to obtain a usable signal.

Recent advances have shown that combining cryofixation with low-temperature Raman imaging can overcome these limitations. In particular, cryogenic conditions reduce diffusion artifacts and allow for longer acquisition times without inducing substantial cellular damage. This approach was recently realized using a cooling stage mounted on a room-temperature microscope, enabling freeze-drying and imaging of samples at liquid nitrogen temperature (77 K). However, the relatively slow freezing process, along with the need for continuous nitrogen gas flow to minimize ice condensation, makes this method suboptimal, compromising sample integrity and introducing mechanical and thermal drift.

To fully harness the advantages of cryogenic Raman imaging of biological samples, we take advantage of shock freezing. Here, we use a custom-built high-vacuum cryogenic shuttle system that enables controlled transfer into and out of a cryogenic microscope operating at liquid helium temperature (4 K). We recently used this system for super-resolution fluorescence microscopy with angstrom precision. In this presentation, we discuss our Raman studies on simple biological specimen maintained in vitreous ice. Our approach paves the way toward high-sensitivity, single-particle cryogenic Raman imaging of vitrified biological systems, with the potential to reveal previously inaccessible biochemical information.

Keywords: Cryogenic Raman imaging, shock-freezing, vitrification, single-particle analysis

[Abstract:0347] [Industrial/Societal Applications]

Raman Assessment of Microplastic Production, Identification and Biotransformation During Human Gastrointestinal Digestion

***Raquel Portela*[1], *Alba Tamargo*[2], *Natalia Molinero Garcia*[2], *Julıan Jımenez Reınosa*[3], *Victor Alcolea-Rodriguez*[1], *Nicolás Coca López*[1], *Jose Fernandez*[3], *Miguel A. Bañares*[1], *M.Victoria Moreno-Arribas*[2]**

[1]*Instituto de Catalisis y Petroleoquimica (ICP), CSIC, Madrid, Spain*
[2]*Instituto de Investigacion en Ciencias de la Alimentacion (CIAL), CSIC, Madrid, Spain*
[3]*Instituto de Ceramica y Vidrio (ICV), CSIC, Madrid, Spain*

Micro- and nanoplastics (MNPs) constitute an emerging environmental and health concern whose assessment requires robust, harmonized analytical approaches supported by representative test/reference materials. Reliable characterization across ecosystems depends on validated instruments, standardized (data) workflows, and adherence to FAIR (Findable, Accessible, Interoperable, Reusable) and open science principles to enable reproducibility, broad adoption, multimodal integration, and machine actionability of Raman datasets. We present ongoing efforts in calibration, data structuring, and comparative algorithm and parameter evaluation, with emphasis on the resulting impacts on automated Raman-based MNP identification. We further report on Raman spectroscopy applied to monitor chemical and structural modifications during the production of test MNPs based on fossil-derived PET [Sci. Rep. 12 (2022) 528] and bio-based PLA [Sci. Total Environ. 902 (2023) 166003] and their use. Polymer crystallinity showed that cryo milled particles are more amorphous and structurally irregular than original pellets, while nano PET generated by dissolution and rapid precipitation is predominantly amorphous. The MNPs were subjected to an in vitro digestion and colonic fermentation model using human faeces to investigate biotransformation processes and their potential links with gut microbiota responses. The exposure experiments revealed material- and donor dependent taxonomic shifts: PET induced a microbial dysfunction, characterized by reduced Bacteroidetes and increased pro inflammatory taxa such as Bilophila, whereas PLA—especially millimetric pellets—favoured beneficial genera including Bifidobacterium, likely supported by microbial enzymatic activities enabling partial PLA degradation. Raman analysis corroborated early microbial colonization and surface modification of PLA. Gastric digestion generated surface pits and pores, and colonic fermentation produced pronounced morphological irregularities and initial amorphous carbon deposits (Raman band at 1601 cm^{-1}). Confocal Raman depth profiles confirmed these as primarily surface phenomena. PET alterations were tracked using Raman intensity ratios 1094/1118 cm^{-1} and 1186/1176 cm^{-1} to assess crystalline–amorphous balance, along with carbonyl band narrowing as an indicator of structural order. Nonetheless, the significance of crystallinity changes remains debated: chain scission may yield shorter fragments capable of recrystallization, while oxidative processes typically disrupt order. Overall, our results suggest that amorphous regions of MNPs are more susceptible to microbial action.

Keywords: microplastics monitoring, algorithm benchmarking, gut microbiota

[Abstract:0348] [SERS/TERS/Plasmonics]

Self-Assembled Core-Shell Nanoparticles for SERS Detection of Fungal Secondary Metabolites

***Mateusz Kasztelan*[1], *Valentina Wolf*[2], *Milda Pucetaite*[1]**

[1]*Laboratory of Biophysics, Wageningen University & Research, Wageningen, The Netherlands, Department of Biology, Lund University, Lund, Sweden*
[2]*Department of Biology, Lund University, Lund, Sweden*

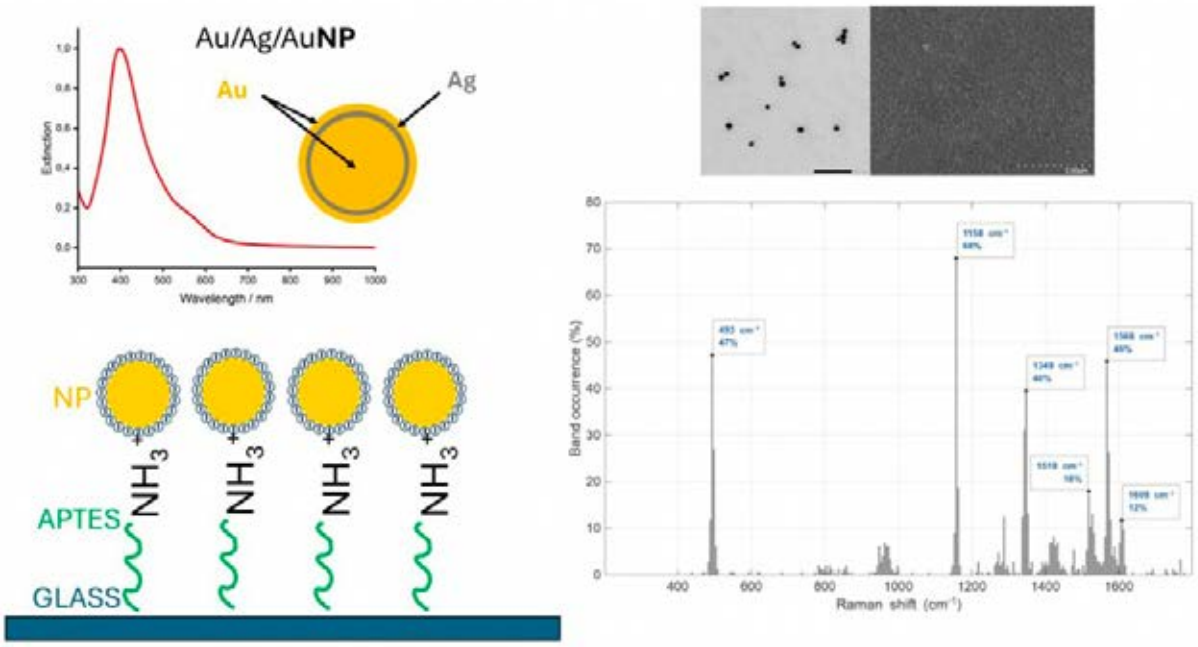
Fungi present in soil continuously interact and compete for nutrients and space. These interactions are largely mediated by secreted molecules known as secondary metabolites. Various compounds are synthesized by fungi to, for example, prevent other species from growing or, vice versa, to detoxify the hazardous chemical environment that the competitors create around them. Despite their importance for ecosystem processes such as carbon cycling and CO_2 emissions from soil, studying these metabolites *in situ* remains challenging. Conventional analytical techniques such as high-performance liquid chromatography or nuclear magnetic resonance provide detailed chemical information but require destructive sample preparation and lack spatial resolution. As a result, they cannot capture where and when metabolites are produced during microbial interactions, which is key for describing their ecological functions.

Raman spectroscopy is a new tool in soil fungal biology and ecology offering a non-destructive alternative that can identify multiple compounds simultaneously based on their molecular "fingerprints". However, its sensitivity is often insufficient for detecting low-abundance metabolites. This limitation can be overcome using surface-enhanced Raman spectroscopy (SERS), where metallic nanostructures amplify the signal. Ideally nanoparticles should be designed in such a way that they not only provide strong enhancement but also do not disturb the living system in *in-vivo* experiment. For that reason, their design must include optimization for biocompatibility.

In this work we present the development of core-shell bimetallic nanoparticles that are self-assembled uniformly on a solid substrate (Figure 1). We evaluated their physical and optical properties using various micro- and spectroscopic methods and their SERS performance using rhodamine 6G and riboflavin as testing compounds. Additionally, we assessed their biocompatibility towards laboratory grown soil fungal cultures and performed preliminary SERS experiments with extracts containing secondary metabolites.

Keywords: fungal secondary metabolites, SERS, core-shell nanoparticles, surface functionalization

Figure 1. Summary of results.



[Abstract:0356] [Non-linear/Time-resolved]

Temperature Dependence of Stimulated Resonant Raman Scattering

***Giovanni Batignani*[1], *Giacomo D'arcangelo*[2], *Gaia De Maria*[1], *Miles Martinati*[1], *Julien Bloino*[2], *Tullio Scopigno*[1]**

[1]*Physics Department, Sapienza University of Rome, Italy*
[2]*Scuola Normale Superiore, Pisa, Italy*

Stimulated Raman spectroscopy (SRS) has been suggested as a potential tool for thermometry to determine the dynamics of mode-specific vibrational energy content during non-equilibrium processes. However, recent studies have highlighted fundamental challenges in utilizing these techniques for this purpose. Specifically, we have shown that in the off-resonant regime, the presence of multiple laser fields introduces quantum pathways that result in destructive interference between Stokes and anti-Stokes processes [Phys. Rev. Lett. 2024, 133, 206902]. This phenomenon ultimately reduces the thermal sensitivity of SRS, nullifying it for harmonic vibrations and temperature-independent polarizability.

In this talk, we address the electronically resonant case, showing how these limitations can be overcome. We demonstrate that under electronically resonant conditions, Franck-Condon transitions alter the relative contributions of these quantum pathways and the resulting interference between them. Consequently, the Raman cross-section and the overall response become inherently temperature-dependent, even within an ideal harmonic model. To validate this framework, we present temperature-dependent measurements performed on a Squaraine dye molecule embedded in a viscous polymer matrix. The resonant SRS spectra acquired over a broad range of temperatures (Fig. 1) reveal how resonance conditions alter the thermal sensitivity. Furthermore, our measurements expose significant anharmonicity effects arising from the coupling between thermally activated low-frequency modes and the higher-frequency vibrations directly probed by the SRS process. These results provide a comprehensive framework for interpreting resonant coherent Raman signals at varying temperatures. Crucially, this understanding establishes a solid foundation for employing SRS as a structural probe in ultrafast pump-probe experiments [Nat. Rev. Methods Primers 2024, 4, 34], enabling the accurate tracking of mode-specific dynamics after a photoexcitation triggers a reaction of interest.

Keywords: Stimulated Raman Scattering, Raman thermometry, Electronic Resonance, Raman Excitation Profile, Anharmonic Couplings

Figure 1

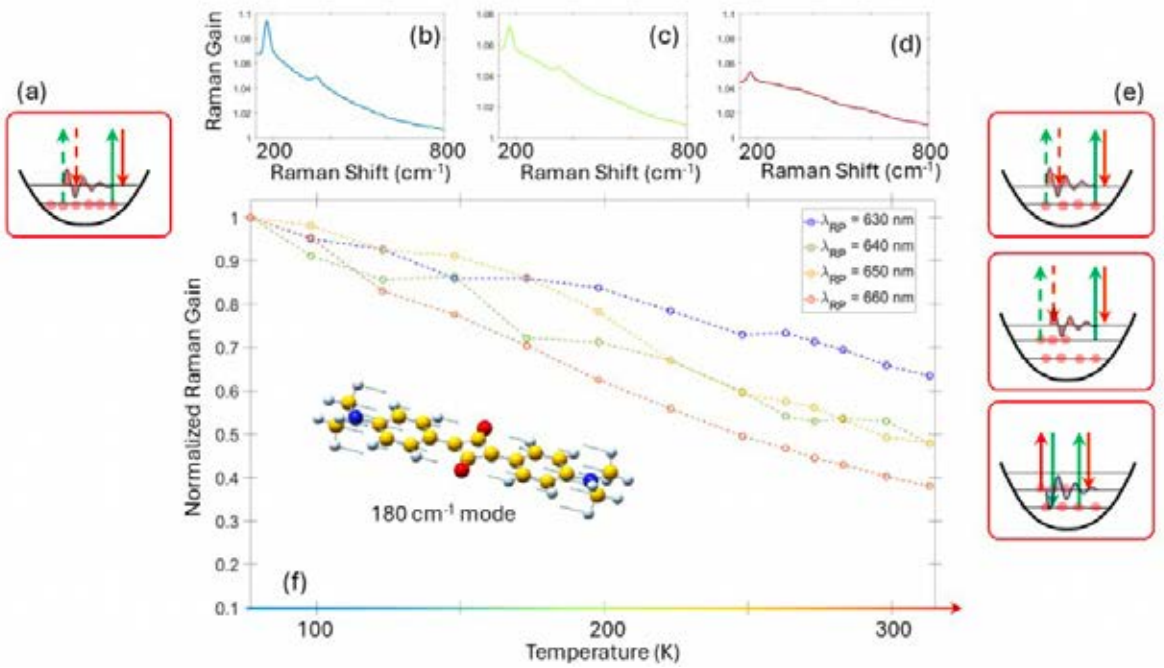


Figure 1: Resonant SRS spectra of Squaraine acquired for different temperatures (b-d) and main underlying pathways responsible for the signal generation (a,e). The normalized SRS cross sections (reported in panel f for a low-frequency breathing mode) reveal a strong dependence on both temperature and resonance condition.

[Abstract:0357] [Non-linear/Time-resolved]

The Origin of the Frequency-Dependence of the OH Stretch Vibrational Lifetimes in Liquid Water – Polarization-Resolved Fs-IR Pump – Stimulated Raman Probe Study

***Marcin Pastorczak*[1], *Aritri Aritri Biswas*[2], *Alexei A. Kananenka*[2]**

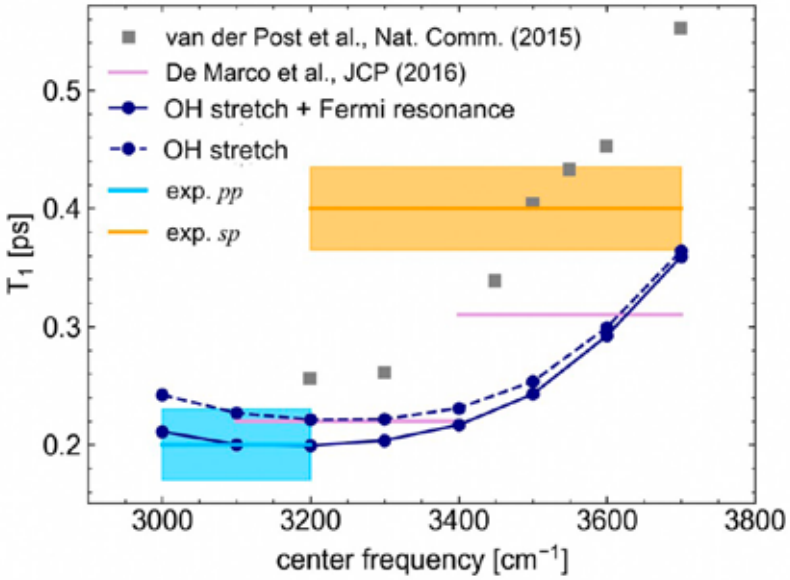
[1]*Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland.*
[2]*Department of Physics and Astronomy, University of Delaware, Newark, Delaware 19716, United States*

The structural heterogeneity of liquid water is among the most debated topics in chemistry. Thus, there is a strong interest in whether such heterogeneity can be observed on the level of water's vibrational lifetimes. The rate of vibrational relaxation of water is crucial, as it affects, e.g., catalysis in aqueous environments and fluorophores' quantum yields. The work by van der Post et al. sparked a vigorous debate over whether water's OH stretch vibrational lifetimes are heterogeneous [van der Post et al. Nat. Comm., 2015] or homogenous [Sung et al. Nat. Comm., 2024].

Here, we used infrared pump-stimulated Raman probe spectroscopy (fs-IR-SRS) to resolve the lifetimes of OH stretching vibrations in liquid water, giving rise to polarized and depolarized Raman signals. We excited liquid water at around 2530 nm, corresponding to the mode at 3950 cm^{-1} comprised of OH stretch and libration. Subsequently, we observed transient stimulated Raman spectra for polarized (*pp*) and depolarized (*sp*) configurations of the Raman pump and the probe. Whereas polarized Raman represents the spectrum of both coupled and decoupled OH oscillators, depolarized Raman is primarily sensitive to decoupled OH groups in water. The lifetime of the OH stretch for the polarized Raman, T^1(pp), was determined here to be 200 fs, in excellent agreement with previous studies. Moreover, we determined, for the first time, the T^1(sp) for the depolarized Raman to be at least two times longer than T^1(pp) (>400 fs), (Fig.1). The depolarized Raman OH stretching band is centered around 3500 cm^{-1}, thus contributing mainly to the blue side of the band, for which a slowed vibrational lifetime has already been observed. The simulations based on quantum-classical line shape theory support experimental findings and predict the increasing dependence of the OH stretch lifetimes on the excitation frequency on the blue side of the spectra. Our results are consistent with the mechanism of OH stretch vibrational relaxation via the bend overtone. The vibrationally decoupled high-frequency OH stretches are off-Fermi resonance with the overtone of the bending mode; thus, their relaxation through OH stretch → HOH bend overtone → HOH bend fundamental mode is much slower.

Keywords: liquid water, vibrational energy relaxations, fs-IR-SRS

Figure 1



Experimental and simulated frequency-dependent OH-stretching lifetimes. Experimentally determined T_1^pp lifetime of 200±30 fs is labelled "pp" and positioned at 3000-3200 cm-1. Experimental relaxation time T_1^sp ~400 fs is labelled "sp" and is positioned at 3200-3700 cm-1 covering the range of depolarized water OH stretching band. Simulated frequency-dependent vibrational energy relaxation times are reported for the calculations that include (solid dark blue) or neglect (dashed dark blue) OH-stretch-HOH bend overtone Fermi resonance. Previously reported experimental results from De Marco et al. [de Marco et al. J Chem Phys, 2016] and van der Post et al [van der Post et al. Nat. Comm., 2015] are shown for comparison.

[Abstract:0359] [SERS/TERS/Plasmonics]

Operando TERS for Analysing Lithium-Transfer Kinetics on Cathode Active Surfaces

***Alice Fiocco*[1], *Joao Lucas Rangel Silva*[1], *Beatrice Laurenti*[2], *Juan Carlos Gonzalez Rosillo*[2], *Francesco Chiabrera*[2], *Fernanda Monteiro Freitas*[2], *Marc Chaigneau*[1], *Alex Morata*[2], *Albert Tarancon*[3]**

[1]*HORIBA France SAS, Palaiseau, France*
[2]*Nanoionics and Fuel Cells, Catalonia Institute for Energy Research (IREC), Barcelona, Spain*
[3]*Catalan Institution for Research and Advanced Studies (ICREA), Barcelona, Spain*

The mechanisms of charge transfer in lithium-ion batteries, as well as the transformations occurring at their electrodes' interfaces, are still object of thorough investigations, with the aim of maximizing the performance and efficiency of the final devices. For this purpose, electrochemical Tip-Enhanced Raman Spectroscopy (EC-TERS) has a great analytical potential, as it allows observing the chemical modifications occurring on the battery materials in operando conditions, i.e. while performing charge/discharge cycles, and at the same time correlating this information with the nanostructure of the sample under investigation. Thanks to the intrinsic multimodality of this technique, it is possible to unveil the structure-activity relationships in the battery components and accordingly improve their conception and design.

The work presented here was carried out in collaboration between HORIBA France and the IREC laboratory in Barcelona, as part of the European project Harvestore, and aimed at correlating the structure of cathode active materials with the kinetic of lithium-ions transfer [*EES Batteries* 2025, 1, 1147]. Notably, for lithium manganese oxide, EC-TERS results were fed to a kinetic model and successfully supported the hypothesis, already presented in the literature [*Nature Communications* 2021, 12, 3085], that ion transfer occurs faster in the grain boundaries of the material. As for lithium iron phosphate, tip-enhanced photoluminescence signals could be used to follow the redox transformation occurring on a grain during cycling, thus proving the versatility and diagnostic power of EC-TERS.

Keywords: TERS, electrochemistry, operando analysis, multimodality

Schematic view of the AFM-based EC-TERS setup

[Abstract:0360] [Novel Approaches]

Advancing Polymer Characterization with Simultaneous Optical Photothermal IR and Raman Micro-Spectroscopy

***Miriam Unger*[1], *Carolin Borbeck*[1], *Heinz Wilhelm Siesler*[2]**

[1]*Photothermal Spectroscopy Corp. GmbH, Muelheim, Germany*
[2]*Department of Physical Chemistry, University Duisburg-Essen, Essen, Germany*

This presentation highlights advances in high-resolution Raman microspectroscopy through its integration with Optical Photothermal Infrared (O-PTIR) spectroscopy for the analysis of complex polymer systems. Raman microspectroscopy provides rich molecular and conformational information, making it a powerful tool for probing chemical and structural heterogeneity at the submicron scale.

The combination of Raman with O-PTIR enables simultaneous, co-located acquisition of Raman and infrared spectra, providing complementary chemical information at submicron spatial resolution. This correlative approach enhances confidence in spectral interpretation and expands the analytical capabilities of vibrational microspectroscopy, particularly in heterogeneous and compositionally complex materials.

The capabilities of this approach are demonstrated across three applications:

(1) Stress-induced transformations in PVDF: Raman and O-PTIR microspectroscopy enable mapping of the α-to-β phase transition and molecular orientation in stretched films, providing detailed insight into strain-induced conformational changes.

(2) Phase separation in PHB/PLA blends: Submicron microspectroscopy resolves the spatial distribution of polymer domains in biodegradable blends, supporting improved understanding of structure–property relationships.

(3) Nylon particle uptake in lung tissue: Correlative microspectroscopy enables detection and quantification of nylon particles in mouse lungs following intratracheal instillation, demonstrating applicability to biologically relevant systems.

These results demonstrate that correlative Raman and O-PTIR microspectroscopy provides a powerful platform for high-resolution, chemically specific characterization across polymer and biological materials.

Keywords: Simultaneous Raman and Submicron IR, O-PTIR, Correlative spectroscopy, Polymer microstructures, Multimodal Spectroscopy

[Abstract:0361] [Planetary/Geosciences]

Raman Laser Spectrometer (RLS) Operations and Scientific Performance for the Rosalind Franklin Mission to Mars

***Guillermo Lopez-Reyes*[1], *Fernando Rull*[1], *Olga Prieto-Ballesteros*[2], *Andoni G. Moral*[3], *Ian Hutchinson*[4], *sylvestre maurice*[5], *Melissa McHugh*[4], *Sofía Julve*[6], *Ana de Dios Cubillas*[2], *Carlos Perez Canora*[3], *Agnes Cousin*[5], *Laura Seoane*[3]**

[1]*ERICA Research Group and LaDIS, University of Valladolid, Spain*
[2]*Centro de Astrobiología (CAB), CSIC-INTA, Torrejón de Ardoz, Spain*
[3]*Departamento de Programas Espaciales, INTA, Torrejón de Ardoz, Spain*
[4]*Department of Physics and Astronomy, University of Leicester, UK*
[5]*IRAP, CNRS, Toulouse, France*
[6]*AstraSpec, Boecillo, Spain*

The Raman Laser Spectrometer (RLS) is part of the scientific payload onboard ESA Rosalind Franklin Mission (ExoMars), aimed at assessing Mars' past habitability and searching for potential biosignatures at Oxia Planum. One of the major scientific strengths of the mission, foreseen for launch in 2028, is its ability to retrieve subsurface samples down to 2m depth, which will be crushed and analyzed at the mineral grain scale through the combined use of the instruments within the Analitycal Laboratory Drawer (ALD): MicrOmega (VIS/IR spectrometer), RLS (Raman spectrometer) and MOMA (GC-LC/MS) instruments.

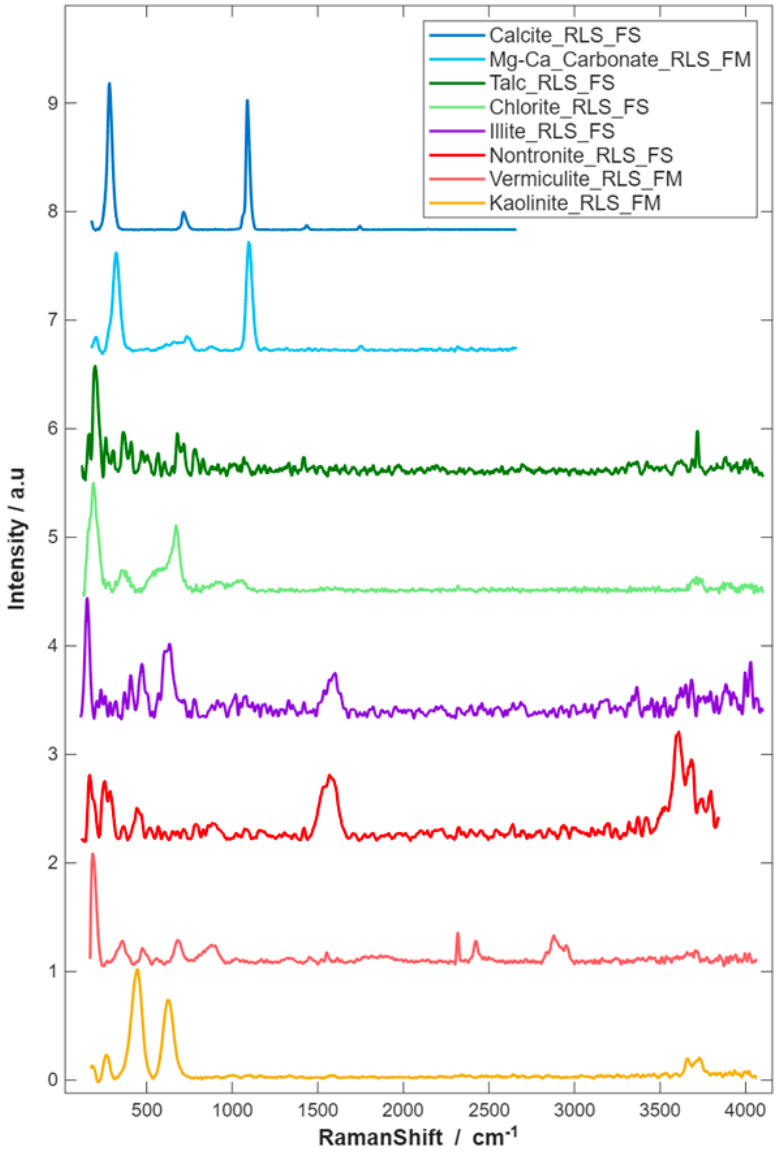
RLS is the Raman instrument of the mission and consists of an optical head focusing the excitation laser and collecting the Raman signal from a ~50 μm spot, a transmission spectrometer covering the 150–3800 cm^{-1} spectral range with an average resolution of ~8 cm^{-1}, and an electronic control unit including the laser source. RLS operation is designed to be fully automated and compatible with rover-driven analytical sequences under Mars mission constraints.

Within the ALD combined science strategy, RLS can perform analyses guided by MicrOmega, targeting selected grains of particular mineralogical interest. Alternatively, RLS could perform automatic acquisitions over 20 to 40 points along the sample. This mode overcomes possible limitations derived from the difference in vibrational activity between IR and Raman and can provide a more representative characterization of powdered samples than guided measurements alone. In addition, RLS can autonomously adapt acquisition parameters to the response of the sample.

The RLS instrument has been extensively tested on both the Flight Model and the Flight Spare using Martian analog samples representative of the mineralogy expected at the landing site, including phyllosilicates, hydrated silica, carbonates, sulfates, and carbon- or organic-bearing compounds, as well as the ExoMars Reference Samples. These samples, specifically selected by the rover team to reproduce mineralogical scenarios of astrobiological relevance to Oxia Planum, are being analyzed in a coordinated manner by the ALD instruments both for operations training and for evaluating the scientific potential of the Rosalind Franklin rover as an integrated analytical system. This contribution will summarize these results and illustrate the expected scientific performance of the instrument

Keywords: Raman spectroscopy, Mars exploration, RLS instrument, Scientific Performance

Example of carbonate and phyllosilicate spectra with RLS



[Abstract:0363] [Non-linear/Time-resolved]

Vibrational Enhancement in $Au_{25}(PET)_{18}$ Nanoclusters Probed by Stimulated Raman Spectroscopy

***Karolina Skała*[1], *Marcin Pastorczak*[1], *Subhradip Kundu*[2], *Arnulf Rosspeintner*[2], *Gonzalo Angulo*[1], *Thomas Bürgi*[2]**

[1]*Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland*
[2]*Department of Physical Chemistry, University of Geneva, Geneva, Switzerland*

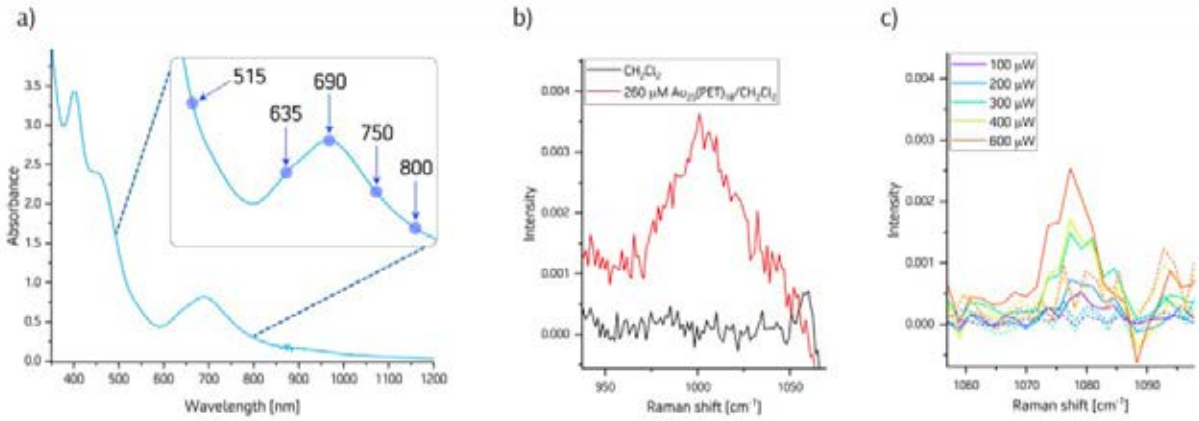
Atomically precise gold nanoclusters (AuNCs), due to their properties lying at the boundary between molecules and nanoparticles, are promising systems for studying structure-dependent optical and vibrational properties, with potential applications ranging from catalysis and photovoltaics to medical imaging and optoelectronics. However, before nanoclusters can be designed for specific applications, it is essential to understand in detail their photophysical properties and the relationship between their structure, electronic states, and vibrational response. Our project focuses on the complex photophysics of these systems and on investigating their vibrational properties in solution.

In this study, we investigate the vibrational properties of the $Au_{25}(PET)_{18}$ nanocluster in solution using stimulated Raman spectroscopy (SRS). Figure 1a shows the electronic absorption spectrum of $Au_{25}(PET)_{18}$ together with the Raman pump wavelengths, selected to probe different resonance conditions. We observe a pronounced pump-wavelength dependence of the vibrational response associated with the PET ligands. Aromatic ring breathing at 1001 cm^{-1}, which is one of the most intense Raman band, was observed for 690 nm Raman pump (Fig. 1b). In contrast, for a Raman pump at 515 nm, we observe a band at approximately 1080 cm^{-1} (Fig. 1c), also originating from PET>s aromatic ring, which is yet only weakly Raman active.

Importantly, the concentration of nanoclusters in the studied solutions (0.26 mM) was below the detection limit for coherent Raman spectroscopy (≈14 mM), which indicates that the observed signals must involve an enhancement mechanism. Since free PET does not absorb in the visible spectral range, the effect cannot be explained by conventional resonance Raman enhancement of the ligand itself. Instead, the results point to a selective enhancement of particular ligand vibrations that depends on the pump wavelength and thus on resonance with specific absorption bands of the nanocluster. In addition, we observe low-frequency vibrational features below 100 cm^{-1}, which also depend on the pump wavelength. These findings provide insight into excitation-wavelength-dependent vibrational enhancement in atomically precise gold nanoclusters.

Keywords: Stimulated Raman Spectroscopy, Atomically Precise Gold Nanoclusters, Enhancement

Fig. 1



(a) Absorption spectrum of $Au_{25}(PET)_{18}$ with the Raman pump wavelengths marked. (b) Stimulated Raman spectra of $Au_{25}(PET)_{18}$ in DCM and neat DCM in the 1000 cm^{-1} region. (c) Stimulated Raman spectra of $Au_{25}(PET)_{18}$ in DCM and neat DCM in the 1080 cm^{-1} region measured at different Raman pump powers. Solid lines: $Au_{25}(PET)_{18}$ in DCM; dashed lines: neat DCM.

Oral Abstracts

[Abstract:0367] [Planetary/Geosciences]

Micro-Raman Based Identification of Impurities in Antarctic Glacier Ice Cores Supported by IC And ICP-MS Analyses

***GAMZE NEŞE ÖZCAN*[1], *FATMA ELIF GENCELI GÜNER*[2]**

[1]*Chemical Engineering Department, Istanbul Technical University, Istanbul, Türkiye*
[2]*Polar Research Center (PolReC), Istanbul Technical University, Türkiye*

Antarctic glacier ice cores preserve valuable information on past environmental and atmospheric conditions, particularly through the characterization of embedded impurities. In this study, Micro-Raman spectroscopy was employed as the primary analytical tool to directly identify solid-phase inclusions within ice cores collected from Horseshoe and Hovgaard regions. Complementary Ion Chromatography (IC) and Inductively Coupled Plasma Mass Spectrometry (ICP-MS) analyses were used to support chemical interpretation and source apportionment.

Micro-Raman analyses, conducted at 532 nm excitation under controlled low-temperature conditions, enabled in situ identification of mineral inclusions at both 5× and 50× magnifications. The results revealed the presence of feldspar, gypsum ($CaSO_4{\cdot}2H_2O$), quartz (SiO_2), and sulfate/nitrate salts such as mirabilite ($Na_2SO_4{\cdot}10H_2O$) and thenardite (Na_2SO_4). Characteristic Raman peaks, including ~463 cm^{-1} (quartz), 980–1040 cm^{-1} (sulfate/nitrate stretching), and broad bands between 3100–3500 cm^{-1} (ice structure), confirmed the mineralogical composition of inclusions. Some inclusions exhibited weak or absent Raman signals, suggesting the presence of Raman-inactive phases such as halite (NaCl), inferred indirectly through chemical data.

IC analysis indicated that Na^+ and Cl^- dominate the ionic composition, confirming strong marine influence, while Ca^{2+}, Mg^{2+}, and K^+ showed mixed marine and crustal origins. ICP-MS results further supported these findings, with enrichment factor calculations revealing marine-derived Na and crustal contributions for elements such as Ba and Mn. Notably, discrepancies between IC and ICP-MS results highlighted micro-scale heterogeneity within the ice matrix, likely due to uneven distribution of inclusions and freeze–thaw fractionation processes.

Importantly, Micro-Raman spectroscopy provided direct mineralogical evidence that could not be obtained solely through bulk chemical analyses. The integration of spectroscopic and chemical techniques demonstrates that Antarctic ice impurities originate from a combination of marine aerosols, terrestrial dust, and long-range atmospheric transport.

This study highlights the critical role of Micro-Raman spectroscopy in resolving impurity composition at the microscale and improving the interpretation of glacial geochemical records.

Keywords: Micro-Raman spectroscopy, Antarctic ice cores, mineral inclusions, ion chromatography, ICP-MS

Oral Abstracts

[Abstract:0368] [Novel Approaches]

Deviations From Inverse-Square Law in Standoff Raman Spectroscopy

***Oleksii Ilchenko*, Mihai Ursta Anghel, Danylo Komisar, Konstantinos Stergiou**

Lightnovo ApS, Birkerod, Denmark

Standoff Raman spectroscopy has evolved from a research technique to a commercial technology over the past decades. Modern systems can acquire high signal-to-noise ratio spectra at distances of 1–10m, while specialized setups with large-aperture collection optics can extend this range to 10–100m. Despite the wide range of applications, the theoretical understanding of how Raman intensity decays with distance remains unclear. Some studies have even reported deviations from the inverse-square law for experiments without focusing sample probes [1]. This motivated us to perform systematic experiments and simulations of Raman intensity as a function of distance for different sample types using standoff Raman spectroscopy setup with collimated laser beam (Figure 1a).

Ray-tracing analysis provides insight into this behavior (Figure 1b). When the sample is close to the spectrograph (0.2m), the Raman signal spreads across the full slit height due to beam propagation after lens L1. At larger distances (e.g., 5m), the signal becomes concentrated near the center of the spectroscopic slit. This effect is confirmed experimentally by CMOS images of benzene Raman signals recorded at various distances (Figure 1c).

Intensity profiles extracted from these images (Figure 1d) were analyzed for different vertical binning values, corresponding to different effective slit heights. For larger slit heights (>1000 μm), both experimental and simulated results follow the expected inverse-square law. However, for smaller slit heights (<1000 μm), the Raman intensity initially increases with distance before decreasing beyond approximately 5 m.

This deviation is caused by the presence of lens L1, which modifies beam propagation and is typically unavoidable in Raman systems. Without L1, the intensity follows the inverse-square law at all slit sizes. Therefore, the apparent deviation arises from system geometry, particularly the use of spectroscopic slits with small height or pinholes.

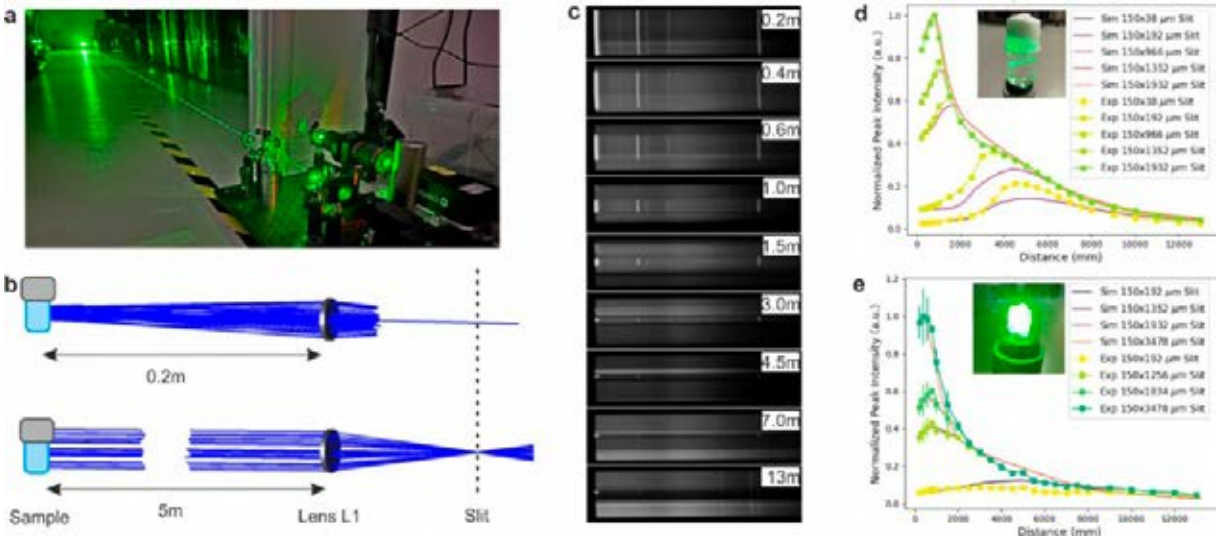
These findings enable more accurate prediction of Raman signal intensity at different distances for standoff geometries with and without laser focusing probes. For example, Figure 1e demonstrates a match between simulation and experiment for highly scattering material such as sulfur crystal, where internal reflections inside the sample significantly increase the scattering area.

References:

[1] E. Languirand, Standoff Raman Semi-Collimated Instrument Evaluation. DEVCOM CBC-TR-1809, 2023.

Keywords: Standoff, Raman spectroscopy, ray tracing

Standoff Raman spectroscopy with collimated laser beam



(a) Photograph of standoff Raman setup, (b) illustration from Zemax Optics Studio of Raman ray tracing to the spectroscopic slit at different distance to the sample (0.2 and 5m), (c) CMOS images of benzene Raman signals recorded at various distances, (d) intensity profiles of Raman signals of benzene versus distance extracted from CMOS images, (e) Raman intensity of sulphur crystal versus distance. Solid lines on Figure 1d,e represent experimental data, dotted lines represent simulation.

Oral Abstracts

[Abstract:0373] [Coherent Raman Imaging]

CARS Endoscopy Through an Ultra-Thin Multi-Core Fiber

***Luca Genchi*[1], *Miriam Maggi*[1], *Federico Vernuccio*[1],**
***Siddarth Sivankutty*[2], *Esben Ravn Andresen*[2], *Hervé Rigneault*[1]**

[1]*Aix-Marseille Univ., CNRS, Centrale Med, Institut Fresnel, Marseille, France*
[2]*Univ. Lille, CNRS, UMR 8523 PhLAM-Physique des Lasers, Atomes et Molecules, F-59000 Lille, France*

Coherent anti-Stokes Raman scattering (CARS) microscopy provides label-free chemical contrast with high specificity and speed, making it a powerful tool for biomedical imaging. However, its implementation in minimally invasive configurations for in vivo applications remains challenging. In addition, the penetration depth of multiphoton imaging in biological tissue is limited to approximately 1 mm. Ultra-thin lensless fiber endoscopes based on multi-mode or multi-core fibers (MCFs) offer a compelling alternative by delivering ultrashort pulses deep into tissue with minimal invasiveness, enabling raster-scanning multiphoton imaging at the tip of a thin optical fiber without additional distal optical elements. In this context, MCFs are particularly attractive because they combine low sensitivity to bending and moderate dispersion, making them well suited for nonlinear imaging over practical fiber lengths.

Here, we present the first implementation of CARS imaging through an ultra-thin MCF endoscope with a distal end below 300 μm. A single spatial light modulator (SLM) simultaneously controls the pump and Stokes beams from a dual-output femtosecond laser, coupling them into different cores of the MCF – avoiding four-wave mixing generated inside the fiber – and applying the phase corrections required to focus at the distal end. Thanks to the low cross-talk between fiber cores, the MCF preserves the so-called memory effect, i.e. the ability to raster-scan the focus by applying global phase tilts at the input facet of the fiber. In the present implementation, scanning is performed with the SLM, although the system is compatible with faster beam-steering approaches based on scanning mirrors. Using spectral focusing, the system also enables selective excitation of different Raman bands within the CH-stretch region.

We demonstrate proof-of-principle CARS imaging of polymer microbeads in a transmission configuration. These results establish the feasibility of coherent Raman imaging through a lensless ultra-thin MCF endoscope. Ongoing work focuses to epi-detection using a double-clad MCF design, toward minimally invasive coherent Raman endoscopy for deep-tissue and in vivo neuroscience applications.

Keywords: lensless endoscope, endoscopy, cars, multi core fiber, wavefront shaping

[Abstract:0374] [Biology/Biomedicine]

Label-Free Raman Spectroscopy in Head and Neck Squamous Cell Carcinoma: From Tumor Biopsies to Therapy Response Monitoring in Patient-Derived Tumor Slice Cultures

***Victor Alcolea-Rodriguez*[1], *Chiara Agrimi*[2], *Nadja Ziller*[3], *Marc Rodriguez-Salazar*[4], *Ulrike Weyer*[3], *Morteza Behrouzitabar*[5], *Giuseppe Antonacci*[6], *Giulio Cerullo*[2], *Dario Polli*[2], *Orlando Guntinas-Lichius*[3], *Anna Mühlig*[3], *Renzo Vanna*[1]**

[1]*CNR-Institute for Photonics and Nanotechnologies (CNR-IFN), P.zza Leonardo Da Vinci 32, 20133 Milan, Italy*
[2]*Politecnico di Milano, Department of Physics, P.zza Leonardo da Vinci 32, 20133 Milan, Italy*
[3]*Department of Otorhinolaryngology, Jena University Hospital, Jena, Germany*
[4]*Datrix SpA, Milan, Italy*
[5]*Università degli Studi di Milano-Bicocca, Milan, Italy 6Specto Photonics, Milan, Italy*
[6]*Specto Photonics, Milan, Italy*

Head and Neck Squamous Cell Carcinoma (HNSCC) diagnosis is predominantly based on Hematoxylin and Eosin (H&E) staining, a technique that lacks intrinsic biochemical specificity. This is often complemented by immunostaining approaches, which offer limited multiplexing capabilities and remain susceptible to inter-observer variability. Furthermore, therapeutic decision-making based on biomolecular determinants of tumor response or resistance remains limited, highlighting the need for robust biomarkers to assess and predict immunotherapy efficacy. In this context, Raman spectroscopy emerges as a promising tool to characterize the biochemical composition of tumors and their microenvironment, improving diagnostic accuracy while enabling therapy monitoring and prediction.

In this work, we present a custom-built spontaneous Raman system (laser excitation at 660 nm) applied to (1) perform chemical imaging of biopsy samples from 34 patients and (2) investigate patient-derived tumor slice cultures (PDTSCs) treated ex vivo with immunotherapy (Durvalumab, anti-PD-L1). The dataset comprises more than 600 Raman maps (120 × 120 pixels), each corresponding to a field of view of 600 × 600 μm. For modeling, pixel-level annotation was achieved using a custom-developed methodology called Multimodal Registration "Sandwich" (MRS), enabling accurate alignment of Raman images with H&E and immunofluorescence reference images.

All spectra were integrated into a single dataset comprising more than 6 million Raman spectra. Tumor biopsies were evaluated using multivariate statistical methods, revealing marked inter-patient biochemical heterogeneity primarily associated with collagen (1070 cm^{-1}), keratin (1246 cm^{-1}), and lipids (2851 cm^{-1}). In parallel, 1D neural networks were employed, achieving a pixel-wise diagnostic accuracy >80% in discriminating tumor from healthy tissue, while the 1246 cm^{-1} band consistently distinguished tumor from stromal regions. Furthermore, global k-means clustering enabled spatial mapping of Raman images, which was compared with H&E images from the same tissue sections. In PDTSC models, the analysis at 4 different timepoints (0-4 days after treatment) showed reductions in DNA- and protein-related spectral features in Durvalumab treated slices compared to controls, indicating therapy-induced biochemical alterations. Overall, Raman spectroscopy demonstrates strong potential as a label-free approach for diagnosis and therapy response monitoring and prediction in HNSCC samples.

Keywords: Head and Neck Squamous Cell Carcinoma (HNSCC), Spectral biomarkers, Tumor biopsies, Therapy monitoring

Oral Abstracts

[Abstract:0379] [SERS/TERS/Plasmonics]

SERS of Stable Radicals and Plasmonically Controlled Radical-Mediated Polymerizations

***Lars Dannenberg*[1], *Naincy Mall*[2], *Helmut Schlaad*[2], *Janina Kneipp*[1]**

[1]*Humboldt-Universität zu Berlin*
[2]*University of Potsdam*

Localized surface plasmon resonances of noble metal nanoparticles are well-known and exploited in Raman spectroscopy due to the high enhancements they can provide for surface-enhanced Raman scattering (SERS). The utilization of gold and silver nanostructures in polymerizations, represents an approach to synthesize polymers in gold nanoparticle solutions, employing light and different plasmonic effects to facilitate and control the growth of polymers.[1] It has been demonstrated that the wavelength- and intensity-dependent activation of the double bond of the allyl mercaptan molecule results in the formation of oligomer chains on silver and gold nanoparticles through a radical mechanism.[1] These reaction products chains can be characterized over time using SERS. However, there is no control of the reactions in relation to chain length and conformation, nor is there any utilization of the reaction product that is formed, as the oligomer molecules are usually bound directly to the plasmonic metal particles by thiols.

Here, we propose to control plasmonic polymerizations through radicals at the surface of plasmonic structures. The involvement of radical species has been proposed by us and others before.[1] In order to understand the interaction of radicals with the plasmonic nanostructures, we studied (2,2,6,6-tetramethylpiperidin-1-yl)oxyl (TEMPO) and corresponding alkoxyamines by SERS. Molecules were modified with different anchoring groups, including thiols, amines, and disulfides, with different binding affinity to the gold nanoparticles. As will be discussed, we found that the formation of the free nitroxide radical is favored at the surface of gold nanoparticles in a concentration-dependent manner and is wavelength-independent.

Acknowledgement

Funding by German Research Foundation (DFG)–CRC/SFB 1636–Project ID 510943930-Project No. B02 is gratefully acknowledged.

References:

[1] L. Dannenberg, H. Schlaad, J. Kneipp, ACS Catalysis 2025, 15, 19328-19342.

Keywords: Photocatalysis, surface-enhanced Raman scattering, radical polymerization, plasmons

[Abstract:0380] [Biology/Biomedicine]

From Cells to Isolated Lipid Droplets: Raman Spectrolipidomics of Treatment Response

***Karolina Chrabąszcz*, Agnieszka Panek, Katarzyna Pogoda**

Department of Biological Physics and Nanospectroscopy, Institute of Nuclear Physics Polish Academy of Science, Krakow, Poland

Radiotherapy is a major treatment strategy for tumors of the peripheral nervous system; however, its effectiveness is often limited by radioresistance and collateral damage to surrounding healthy tissues. Increasing evidence indicates that lipid metabolism and lipid droplet remodeling, plays an important role in cellular responses to ionizing radiation. Cannabidiol (CBD), a bioactive compound with both anticancer and neuroprotective properties, has therefore emerged as a potential modulator of radiological response. Nevertheless, the molecular mechanisms underlying CBD-mediated changes in radiosensitivity remain poorly understood.

In our previous studies, multimodal vibrational spectroscopy, revealed significant alterations in lipid composition in cells exposed to CBD and ionizing radiation. To investigate lipid dynamics with greater chemical specificity, we introduced deuterium-labeled lipid probes as spectroscopically active sensors. Raman and infrared spectroscopic characterization of these probes provides a basis for semi-quantitative analysis of lipid uptake, redistribution, and metabolic transformation in cellular systems.

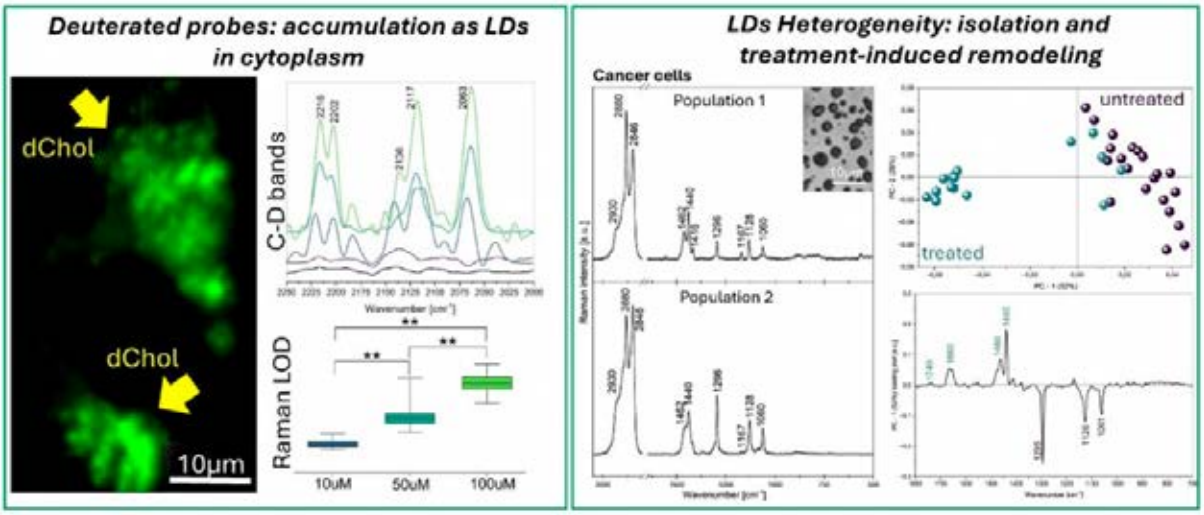
Building on this approach, deuterated cholesterol (dChol) was applied as a molecular probe to monitor nanoscale cholesterol remodeling in peripheral glial cells treated with CBD. Multimodal Raman, FT-IR, and AFM-IR spectroscopies enabled spatially resolved visualization of cholesterol uptake, esterification, and membrane integration, revealing that the sequence of CBD exposure relative to lipid incorporation activates distinct metabolic pathways (Fig. 1). Because lipid metabolism in cells represents a complex interplay of multiple compartments, we further extended this investigation to isolated lipid droplets (iLDs), key organelles involved in metabolic regulation and stress adaptation. Raman analysis of iLDs isolated from normal Schwann cells and malignant peripheral nerve sheath tumor (MPNST) cells demonstrated pronounced biochemical heterogeneity and treatment-dependent remodeling of lipid droplet cargo (Fig. 1). CBD treatment, irradiation, and their combination induced distinct lipid compositional changes, highlighting lipid droplets as sensitive reporters of metabolic reprogramming associated with radiosensitization.

Together, these results establish a spectrolipidomic framework based on Raman and infrared spectroscopy for probing lipid metabolism across molecular, cellular, and suborganelle levels. This approach provides new insights into lipid-mediated mechanisms of radiation response and opens new avenues for spectroscopy-based biosensing of metabolic adaptations in cancer therapy.

Acknowledgement: This work was supported by the National Science Centre of Poland under research project no 2023/51/D/ST4/01686.

Keywords: spectrolipidomics, lipids, radioresistance, lipid droplets

Figure 1.



(Left) Deuterium-labeled lipid probes accumulate in cells and localize within cytoplasmic lipid droplets (LDs); the detection limit is determined from the C-D vibrational bands. (Right) Raman spectroscopy of isolated lipid droplets (iLDs) reveals lipid droplet population heterogeneity and treatment-induced lipid remodeling.

[Abstract:0382] [Industrial/Societal Applications]

Smaller Plastics, Bigger Risks: Correlative Raman and O-PTIR Microspectroscopy for High-Confidence Identification of Submicron Microplastics

***Carolin Borbeck*[1], *Miriam Unger*[1], *Mustafa Kansiz*[2], *Eoghan Dillon*[2]**

[1]*Photothermal Spectroscopy Corp GmbH, Landgrafenstr. 12, 45476 Mülheim an der Ruhr, Germany*
[2]*Photothermal Spectroscopy Corp, 325 Chapala Street, Santa Barbara, CA 93101, USA*

Microplastic (MP) contamination has become a global environmental and health concern, with particles now detected in water, air, soil, and biological systems. These particles can enter the human body through ingestion or inhalation, where submicron microplastics and nanoplastics (<1 μm) are of particular concern due to their ability to cross biological barriers and accumulate in tissues.

Raman microspectroscopy is a key analytical technique for MP characterization, offering high spatial resolution and strong chemical specificity for small particle analysis. However, in complex sample matrices, fluorescence interference, weak signals, and susceptibility to colored particles can generate poor-quality spectra or complicate spectral interpretation. This can include potential misidentification of long-chain molecules such as stearates as polyethylene (PE). Complementary vibrational approaches can enhance analytical confidence, particularly at the smallest size scales relevant to biological uptake and toxicity.

Optical Photothermal Infrared (O-PTIR) microspectroscopy addresses these challenges by enabling true submicron infrared spectroscopic spatial resolution (<500 nm), generating IR spectra – collected in reflection mode – that are fully comparable and compatible with FTIR transmission/ATR spectra. More importantly, O-PTIR allows simultaneous, co-located Raman measurements from the same particle, enabling direct correlation of complementary chemical information. This enhances confidence in particle characterization.

We have developed automated workflows combining Raman microspectroscopy with O-PTIR for the detection and chemical characterization of micro- and nanoplastics, with results on particles as small as 250 nm. Following optical and cross-polarized light microscopy, optionally supported by fluorescence imaging, particles of interest are automatically targeted for fully co-localized O-PTIR and Raman analysis. Case studies demonstrate how this approach enables high-confidence detection, identification, and spatial mapping of micro- and nanoplastics in environmental and biological samples, including clear differentiation of polyethylene from structurally similar long-chain species such as stearates.

This correlative approach enhances the analytical power of Raman microspectroscopy, enabling more reliable characterization of submicron plastic particles in complex, real-world samples.

Keywords: Multimodal imaging, Optical Photothermal Infrared (O-PTIR), Microplastics, Nanoplastics, simultaneous Raman spectroscopy, Submicron imaging

[Abstract:0384] [Coherent Raman Imaging]

Multimodal Nonlinear Raman Imaging for Label-Free Histology of Head and Neck Tumor Microarrays

***Marco Da Ros*[1], *Francesco Di Pasquale*[1], *Martino Scoca*[1], *Victor Alcolea-Rodriguez*[1], *Nadja Ziller*[3], *Marc Rodriguez-Salazar*[4], *Ulrike Weyer*[3], *Giulio Cerullo*[1], *Orlando Guntinas-Lichius*[3], *Anna Mühlig*[3], *Renzo Vanna*[2], *Dario Polli*[1]**

[1]*Department of Physics, Politecnico di Milano, Milan, Italy.*
[2]*CNR-Institute for Photonics and Nanotechnologies (CNR-IFN), Milan, Italy*
[3]*Department of Otorhinolaryngology, Jena University Hospital, Jena, Germany*
[4]*Datrix SpA, Milan, Italy*

Head and Neck Squamous Cell Carcinoma (HNSCC) diagnosis relies on tissue biopsies, where rapid and reliable screening of large cohorts, such as Tumor Microarrays (TMAs), is essential for translational research. Conventional histopathology based on Hematoxylin and Eosin (H&E) staining, often complemented by immunofluorescence (IF), remains the gold standard. However, these methods provide limited intrinsic biochemical contrast and are prone to observer variability. Consequently, there is a growing need for fast, label-free imaging strategies offering objective biochemical characterization.

To address this, we present a novel multimodal nonlinear optical (NLO) laser-scanning microscope (Fig. 1), powered by a single, compact tunable near-infrared femtosecond fiber laser. This platform seamlessly integrates Stimulated Raman Scattering (SRS), Coherent Anti-Stokes Raman Scattering (CARS), Second-Harmonic Generation (SHG), and Two-Photon Excitation Fluorescence (TPEF). This custom setup enables comprehensive, label-free imaging of complex biological samples, capturing rich chemical, structural, and metabolic information in parallel.

We employed this setup to analyze TMAs from 20 HNSCC patients (Fig. 2). To efficiently capture these large areas (1.2 mm field of view), we implemented strip mosaicking with image stitching and supported by an automated autofocus system. To accurately correlate our label-free vibrational data with clinical standards, we performed pixel-wise annotation using a custom Multimodal Registration "Sandwich" approach, aligning our NLO images with adjacent H&E and IF references.

A key capability of our platform is performing rapid, high-resolution SRS imaging across both the high-wavenumber C-H stretching bands (50 µs pixel dwell time) and the technically challenging biochemical fingerprint region (400 µs pixel dwell time). By combining this fingerprint-rich SRS data with robust C-H signals, alongside structural SHG and TPEF, we capture a comprehensive biochemical picture. This synergistic approach enhances our ability to identify distinct signatures that differentiate tumoral tissue from surrounding healthy stroma. Ultimately, this multimodal dataset lays the groundwork for training robust predictive models and exploring the reconstruction of objective, false-color H&E-like images directly from NLO signals.

Keywords: Stimulated Raman Scattering, Tumor Microarray, Label-free imaging, Head and neck squamous cell carcinoma, Multimodal microscopy

Label-free multimodal imaging of an HNSCC TMA tissue section

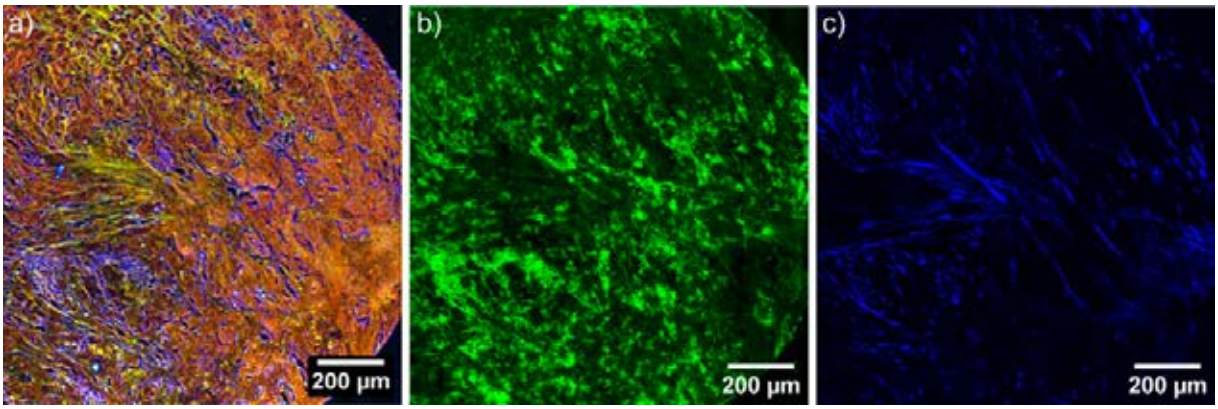


Figure 2. a) SRS false-color composite mapping distinct biochemical components: proteins (red), lipids (green), and DNA (blue). Complementary NLO modalities acquired in parallel include b) TPEF, detailing metabolic and morphological features, and c) SHG, mapping the collagen networks of the tumor microenvironment.

Schematic representation of the multimodal microscope

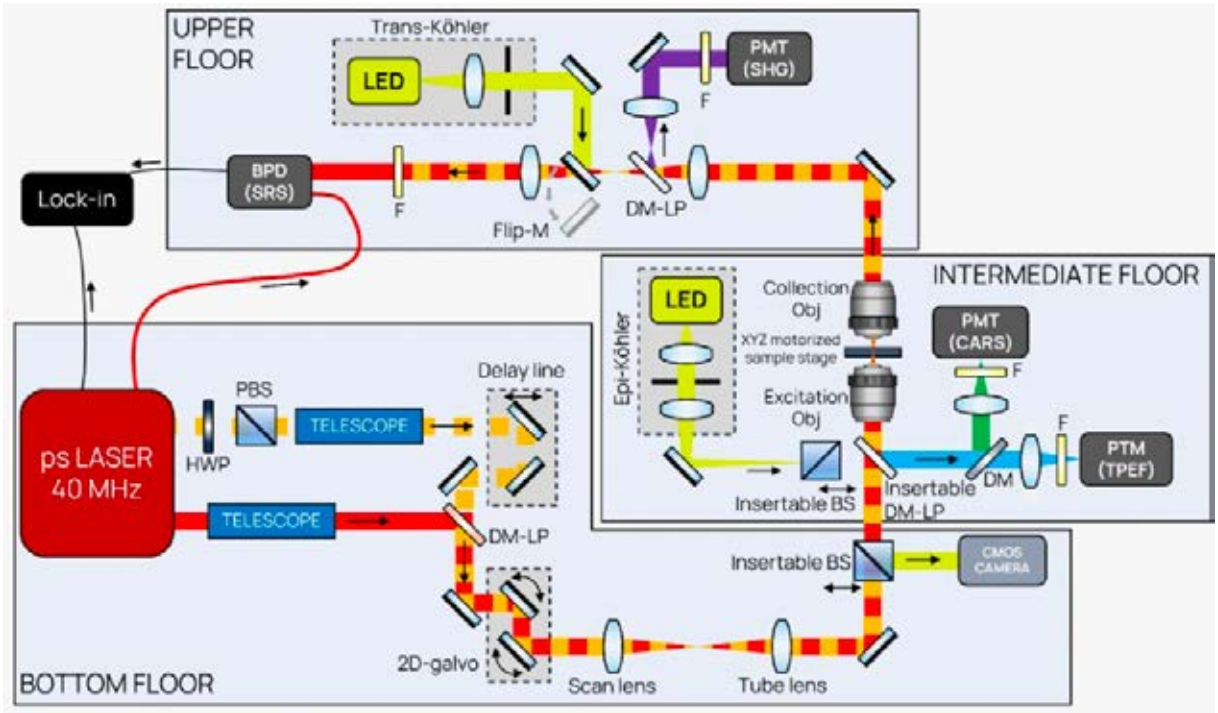


Figure 1. HPW: half-wave plate. BS (PBS): (polarizing) beam splitter. DM-LP: dichroic mirror long pass. F: filter. M: mirror. Red line: pump. Yellow line: Stokes. Green line: CARS. Cyan line: TPEF. Purple line: SHG.

[Abstract:0389] [Novel Approaches]

Miniature Raman Spectrometer with Tunable Laser for Minerals Research

***Nicolai Jonathan E. Jacobsen*, Andrii Kutsyk, Yurii Pilhun, Oleksii Ilchenko**

Lightnovo ApS, Birkerød, Denmark

In handheld Raman measurements of minerals, small variations in laser excitation wavelength can strongly affect spectra. Many minerals exhibit fluorescence with narrow peaks, making it difficult to distinguish fluorescence from Raman scattering. Fluorescence features shift with excitation wavelength, while Raman peaks remain fixed, complicating comparisons across instruments or use of spectral libraries. Approaches to address this include laser wavelength stabilization, calibration with an off-axis reference channel [1], and shifted excitation Raman difference spectroscopy (SERDS). Here, we demonstrate a combined approach using (1) SERDS and (2) laser wavelength stabilization via an off-axis reference channel, allowing full separation of fluorescence from the Raman response.

1. Our miniature Raman spectrometer integrates a polystyrene reference channel (Figure 1a) to monitor laser wavelength during acquisition, typically tuning within 4-5 nm at a linewidth of 0.2-0.3 nm. For SERDS, the laser power was tuned to induce controlled shifts in excitation wavelength. Figure 1b shows zircon spectra at different laser powers (785-790 nm excitation) using a 785 nm system, illustrating that fluorescence peaks shift with wavelength while Raman peaks remain fixed. This dataset enabled reconstruction of separate Raman and fluorescence spectra (Figure 1c).

2. For spectral database creation, a fixed excitation wavelength is preferable. We implemented software-based laser stabilization in a miniature Raman spectrometer with a 660 nm laser. Using the built-in reference channel [1], the excitation wavelength is measured (660-665 nm) and used to adjust the laser current. A proportional-integral (PI) control loop compensates for variations due to current, temperature, and device-specific factors, maintaining the wavelength near the defined target (Figure 1d).

Wavelength stabilization is achieved within 30 seconds, enabling reliable identification of minerals containing both Raman and fluorescence features across different devices (Figure 1e).

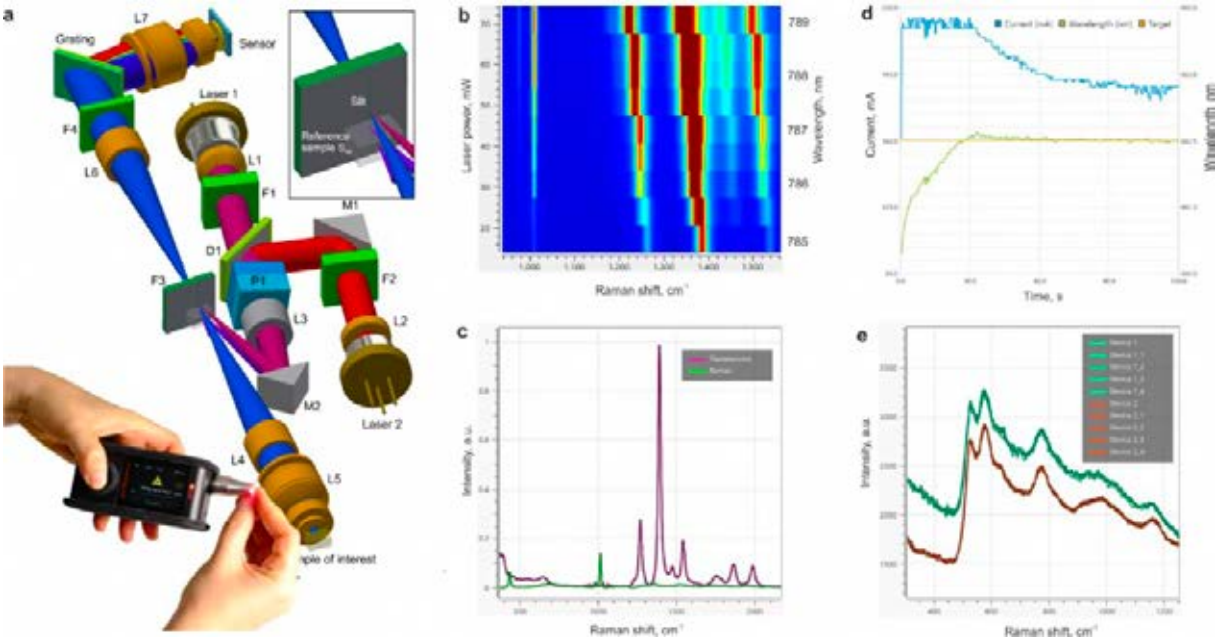
This combined approach offers an efficient way to study and differentiate Raman and fluorescence spectra in mineralogy, supporting accurate mineral identification within the compact form factor of miniature Raman spectrometers.

References:

[1] O. Ilchenko et al, Optics miniaturization strategy for demanding Raman spectroscopy applications, Nat. Commun. 15 (2024) 3049.

Keywords: Raman spectrometer, tunable laser, SERDS, minerals

Miniature Raman spectrometer with tunable laser



(a) Raman setup with built-in reference channel, (b) spectra of zircon obtained at different laser power/ wavelength that correspond to laser tuning range 785-789 nm, (c) SERDS reconstruction of Raman and fluorescence spectra of zircon, (d) laser wavelength stabilization using PI controller, (e) fluorescence spectra of glass obtained on different miniature Raman devices with PI stabilized wavelength at 662.5 nm.

[Abstract:0390] [Materials]

Study of Polymorphism in the Family of Guanidine-Based Molecular Crystals for Nonlinear Optics

***Ivan Němec*[1], *Irena Matulková*[1], *Martin Zábranský*[1], *Ivana Cisarova*[1], *Róbert Gyepes*[1], *Jiri Skopalik*[1], *Petr Nemec*[2]**

[1]*Department of Inorganic Chemistry, Faculty of Science, Charles University, Prague, Czech Republic*
[2]*Department of Chemical Physics and Optics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic*

Within the family of the actually prepared and studied materials for nonlinear optics (NLO), molecular crystals represent a very promising group of compounds with wide application potential. This class of compounds (i.e. salts and cocrystals) benefits from the presence of highly polarisable organic molecules (carriers of NLO properties) whose proper crystal packing is achieved through the incorporation of hydrogen-bonded co-crystallisation partners. Their applications, which include the generation of new laser frequencies, signal processing, optical communications, all-optical switching, or optical power limiting, are based on many NLO effects such as SHG - Second Harmonic Generation, THG - Third Harmonic Generation, cascaded self-frequency doubling and tripling, and the processes associated with Stimulated Raman Scattering (SRS).

A necessary condition for the existence of individual NLO effects is the appropriate symmetry of prepared crystals. For example, second-order nonlinear optical effects (such as SHG) require non-centrosymmetric crystal packing; thus, phase analysis, the study of polymorphism, and phase transitions are among the key tasks in characterising these materials.

This contribution focuses on the study of polymorphism and the explanation of the observed phase transition mechanisms in the family of molecular crystals containing "Y-aromatic" species, such as guanidine and its derivatives (e.g., aminoguanidine and N-guanylglycine) in combination with selected anions, using spectroscopic, diffraction and calorimetric methods. In addition to temperature-dependent Raman spectroscopy, an essential experimental technique, results of FTIR, X-ray diffraction, SHG and DSC studies were employed.

Acknowledgements: Advanced Multiscale Materials for Key Enabling Technologies (AMULET) project, supported by the Ministry of Education, Youth, and Sports of the Czech Republic (project No. CZ.02.01.01/00/22_008/0004558) is gratefully acknowledged.

Keywords: molecular crystals, NLO, phase transition, polymorphism, Raman spectroscopy

[Abstract:0392] [SERS/TERS/Plasmonics]

Probing a Reactive Alkyne Centre Aligned by a Rigid Molecular Tripod by Single-Molecule TERS for Electric Field-Induced Chemistry

***Sebastian Schlücker*[1], *Simon Mennicken*[1], *Gang Li*[2], *Till Reichenauer*[1], *Luyao Zhu*[2], *Gebhard Haberhauer*[2], *Zhen Chao Dong*[1]**

[1]*Department of Chemistry, University of Duisburg-Essen, Essen, Germany*
[2]*University of Science and Technology of China, Hefei, Anhui, China*

Electric-field induced chemistry is an exciting and elegant way of controlling chemical reactions via oriented external electric fields.[1] We selected terminal alkynes as a model system for reactive centres.[2] The latter must fulfil several conditions for use in electric field-induced chemistry: (i) stability in the presence of high electric field strengths on the order of 1 V/Å, (ii) defined orientation relative to the external electric field, and (iii) immobility on the underlying metal surface for continuous observation in situ. These conditions are met by reactive centres conjugated to triphenylmethane-based rigid molecular tripods for strong immobilization on gold surfaces (multivalency) and a defined orientation perpendicular to the gold surface due (sp3-hybridized core). We synthesized and characterized alkyne-terminated tripods using single-molecule TERS under ultra-high vacuum (UHV) at low temperatures (LT). STM imaging and UHV-LT-TERS spectra confirm a nearly upright orientation of individual tripods, characterized by a dominant C≡C stretching peak in the Raman-silent region (see Figure 1). Overall, our results demonstrate the ability to probe chemically reactive centres under the influence of intense external electric fields using a combination of rigid molecular tripods, STM and TERS.

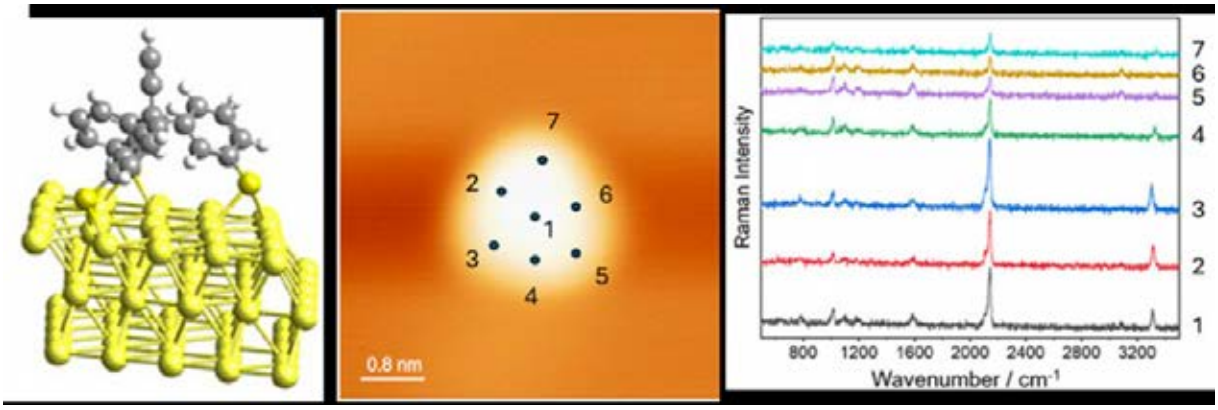
References:

[1] S. Shaik, D. Danovich, K. D. Dubey, and T. Stuyver, in Effects of Electric Fields on Structure and Reactivity New Horizons in Chemistry, ed. S. Shaik and T. Stuyver, The Royal Society of Chemistry, 12-70 (2021).

[2] S. Mennicken, G. Li, L.Y. Zhu, D. Schäfer, T. Reichenauer, S. Mehrparvar, N. Choi, Y. Zhang, G. Haberhauer, Z.-C. Dong & S. Schlücker. Probing a Reactive Alkyne Center Aligned via a Triphenylmethane Tripod on Au(111) for Electric Field-Induced Chemistry by STM and TERS. Small, 22(7), e09467 (2026).

Keywords: E-field catalysis, terminal alkyne, reactive center, rigid tripod, UHV-LT-TERS

Figure 1.



Characterization of an alkyne-terminated rigid tripod on Au(111). Left: DFT-optimized structure. Middle: STM image showing intramolecular TERS measurement points (1–7). Right: Corresponding intramolecular TERS spectra.

[Abstract:0395] [Biology/Biomedicine]

Vibrational Probing of the Glycosaminoglycan Structure-Function Relationship Through Physicochemical Perturbation

***Gergo Peter Szekeres*[1], *Jan Horlebein*[2]**

[1]*Department of Biology, Chemistry, Pharmacy, Freie Universität Berlin, Berlin, Germany; Department of Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*
[2]*Department of Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany*

Glycosaminoglycans (GAGs) are linear polysaccharides that play a crucial role in physiological processes due to their strong polyanionic character and varying sulfation pattern.[1] While significant contributions have been made to their vibrational spectroscopic characterization, these still often focus on compositional analysis, and do not usually look beyond purity assessment. Therefore, a systematic vibrational spectroscopic investigation of GAGs can reveal unique features that allow the understanding of GAG structural dynamics at the levels established for proteins and nucleic acids.

In this work, aqueous GAG samples (e.g., chondroitin sulfate variants and heparin) were studied by polarization-resolved Raman spectroscopy. The samples were probed under varying environmental conditions, including a broad temperature range and the presence of different bivalent cations. The cation identity directly modulates local sulfate coordination geometry and backbone conformational order, revealing structural differences between GAG classes that otherwise would remain obscured. Furthermore, complementary linear and nonlinear vibrational spectroscopy techniques both in solution and in the gas phase were employed, providing highly specific insight into local structural features, macromolecular organization, and interfacial behavior.[2,3]

References:

[1] G. P. Szekeres, ChemBioChem 26, e202500418 (2025)

[2] J. Riedel, J. Am. Chem. Soc. 145, 7859-7868 (2023)

[3] G. P. Szekeres, Phys. Chem. Chem. Phys. 23, 13389-13395 (2021)

Keywords: Glycosaminoglycans, GAGs, Raman spectroscopy, perturbation

[Abstract:0396] [Industrial/Societal Applications]

Discrimination of Regional Honey Samples From Northeastern Türkiye Using Raman Spectroscopy

***Akif Goktug Bozkurt*[1], *Leyla Demirci*[2]**

[1]*Department of Food Processing, Ardahan University, Ardahan, Turkiye*
[2]*Department of Advanced Technologies, Ardahan University, Ardahan, Turkiye*

The authentication of honey in terms of geographical origin and production characteristics is of increasing importance for quality assurance and the prevention of food fraud. In this study, Raman spectroscopy combined with multivariate analysis was employed to investigate the compositional variability of honey samples produced predominantly by the Caucasian honeybee (*Apis mellifera caucasica*) in Northeastern Türkiye. A total of 33 honey samples were collected from the central district and five different districts of Ardahan province, along with additional samples from neighboring provinces, Kars and Artvin. The dataset spans two consecutive production years (2024–2025), enabling evaluation of both spatial and temporal variability in honey composition. Raman spectra were acquired using a 785 nm excitation laser, with measurements performed in liquid sample cuvettes under standardized conditions to ensure reproducibility and minimize external variability. Prior to analysis, spectral data were preprocessed baseline correction and normalization procedures. Principal Component Analysis (PCA) was applied as an unsupervised chemometric approach to reduce data dimensionality and identify underlying patterns within the dataset. The PCA results showed that the first principal component (PC1) accounted for 69.66% of the total variance, while the second principal component (PC2) explained 12.18%, yielding a cumulative variance of 81.84%.

The PCA score plot revealed a clear clustering of Ardahan samples, suggesting compositional consistency associated with the dominance of *Apis mellifera caucasica* and relatively similar floral sources. In contrast, samples from Kars and Artvin displayed broader dispersion, indicating greater variability in botanical origin and environmental conditions. Moreover, the presence of outliers along PC2 suggests that interannual differences between the 2024 and 2025 harvests may influence honey composition, potentially due to climatic fluctuations and nectar source variability. These results demonstrate that Raman spectroscopy, combined with PCA, provides a rapid, non-destructive, and reagent-free method for differentiating honey based on both geographical origin and production year. Future studies should incorporate supervised classification techniques and expanded datasets to further improve classification performance and model robustness.

Keywords: Principal Component Analysis (PCA), Apis mellifera caucasica, Honey authentication, Food quality control

[Abstract:0397] [Materials]

Ultrastability and Hyperageing in Amorphous Materials: Polarization Resolved Stimulated Raman Spectroscopy of Fossil Amber

Giovanni Batignani[1], Emanuele Mai[1], Miles Martinati[1], Neethish Madathiparambil Mohanan[1], Daniele Cangialosi[2], Marcos Pimenta[3], Miguel Ángel Ramos[4], Tullio Scopigno[1]

[1]*Dipartimento di Fisica, Sapienza Università di Roma, Rome, Italy*
[2]*Centro de Física de Materiales, (CSIC–UPV/EHU), San Sebastián, Spain*
[3]*Departamento de Física, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil*
[4]*Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain*

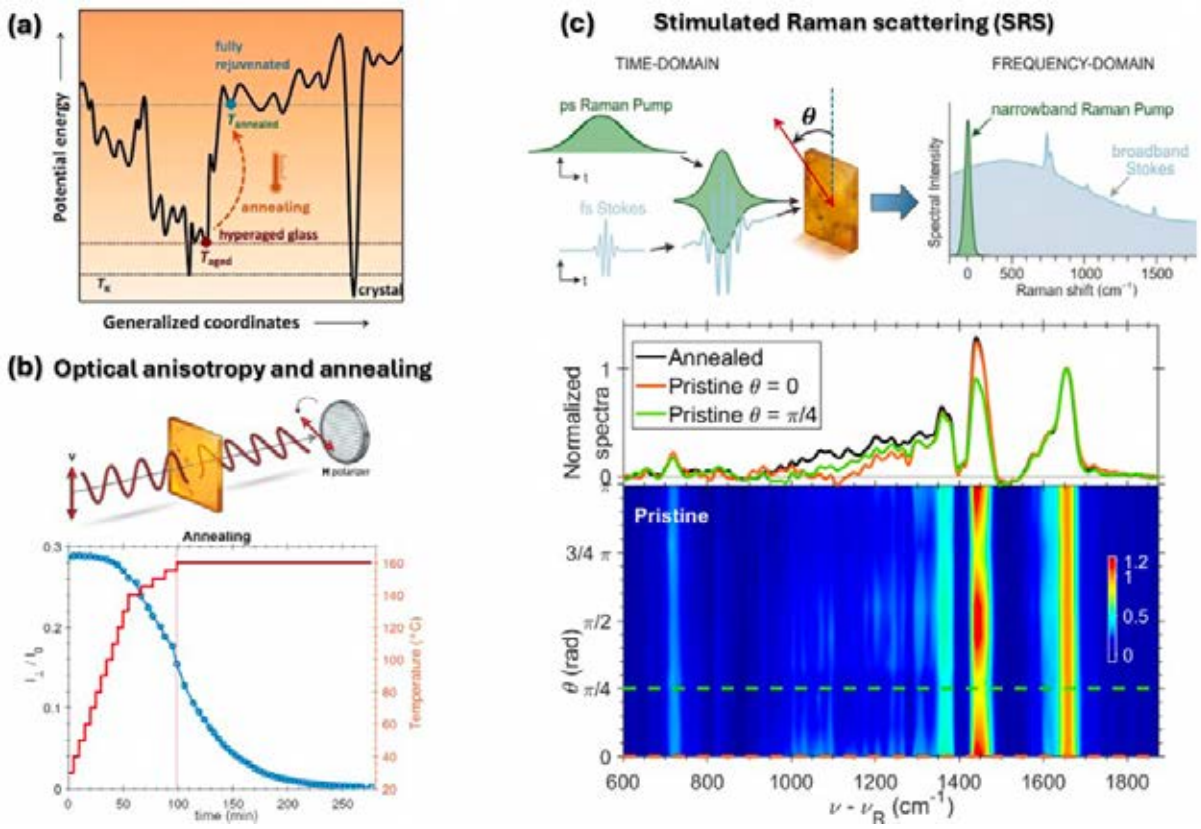
The fundamental physical mechanisms governing the long-term thermodynamic stabilization of complex glasses remain deeply obscure. In this context, geologically hyperaged amber emerges as a unique natural laboratory to investigate the structural order induced by millennial aging in the vitreous state. In such extremely aged systems, the connection between structural disorder and the potential energy landscape becomes apparent. Over geological timescales, these materials undergo a subtle densification—distinct from hydrostatic compression—and associated ordering of the elastic matrix *[J. Phys. Chem. Lett. 2019, 10, 427–432]*, while low-temperature vibrational anomalies like the boson peak remain stable *[Phys. Rev. Lett. 2014, 112, 165901]*. Thermal annealing irreversibly erases this thermal history and its ultraslow energy landscape exploration, returning the aged glass to a less stable, rejuvenated configuration (Fig.1a).

To uncover the microscopic mechanisms of this macroscopic stabilization, we conducted a comprehensive experimental investigation comparing pristine hyperaged amber with its rejuvenated counterpart. We employed complementary analytical techniques, including optical polarimetry, differential scanning calorimetry, X-ray diffraction and, most importantly, polarization-resolved stimulated Raman spectroscopy.

The critical initial observation of macroscopic optical birefringence in hyperaged amber samples -a feature that is completely lost upon thermal annealing (Fig.1b)- paved the way for more specific probe of these geological structural rearrangements, which has been achieved through *polarized stimulated Raman spectroscopy (SRS)*. By systematically analyzing the polarization dependence of the stimulated Raman spectra, we successfully tracked the hidden orientational order within the amorphous network (Fig.1c). Crucially, the polarized SRS approach provides a pronounced, mode-specific sensitivity, which enabled us to decouple the orientational behavior of C-C backbone vibrations from that of C-H stretching modes along the polymer chain. These findings provide unprecedented microscopic insight into local structural anisotropies originating from extreme aging, shedding new light on the slow dynamics and fundamental physical mechanisms ruling the stabilization of complex glassy materials.

Keywords: Polarized Raman Spectroscopy, Hyperaged Amber, Glasses, Anisotropy, Stimulated Vibrational Spectroscopy

Figure 1



(a) Thermal annealing erases the millennial stabilization of hyperaged glasses. (b) Pristine hyperaged amber exhibits optical birefringence, which disappears upon heating above the glass transition. (c) Polarized SRS reveals periodic modulations of specific Raman bands with sample orientation (θ) exclusively in the pristine sample, exposing age-induced local structural anisotropies along distinct molecular vibrations.

[Abstract:0398] [Non-linear/Time-resolved]

Broadband Stimulated Raman Scattering on Methylene Blue: Probing Equilibrium and Excited State Properties

Giovanni Batignani[1], Giacomo D'Arcangelo[2], Gaia De Maria[3], Julien Bloino[4], Tullio Scopigno[5]

[1]Dipartimento di Fisica, Università di Roma "La Sapienza", Roma I-00185, Italy
[2]Scuola Normale Superiore, Piazza dei Cavalieri 7, Pisa 56126, Italy, Applied and Laser Spectroscopy Laboratory, Institute of Chemistry of Organometallic Compounds, Research Area of National Research Council, Pisa 56124, Italy
[3]Dipartimento di Fisica, Università di Roma "La Sapienza", Roma I-00185, Italy, Dipartimento di Scienze di base e applicate per l'Ingegneria, Università di Roma "La Sapienza", Roma I-00185, Italy
[4]Scuola Normale Superiore, Piazza dei Cavalieri 7, Pisa 56126, Italy
[5]Dipartimento di Fisica, Università di Roma "La Sapienza", Roma I-00185, Italy, Graphene Labs, Istituto Italiano di Tecnologia, Genova I-16163, Italy

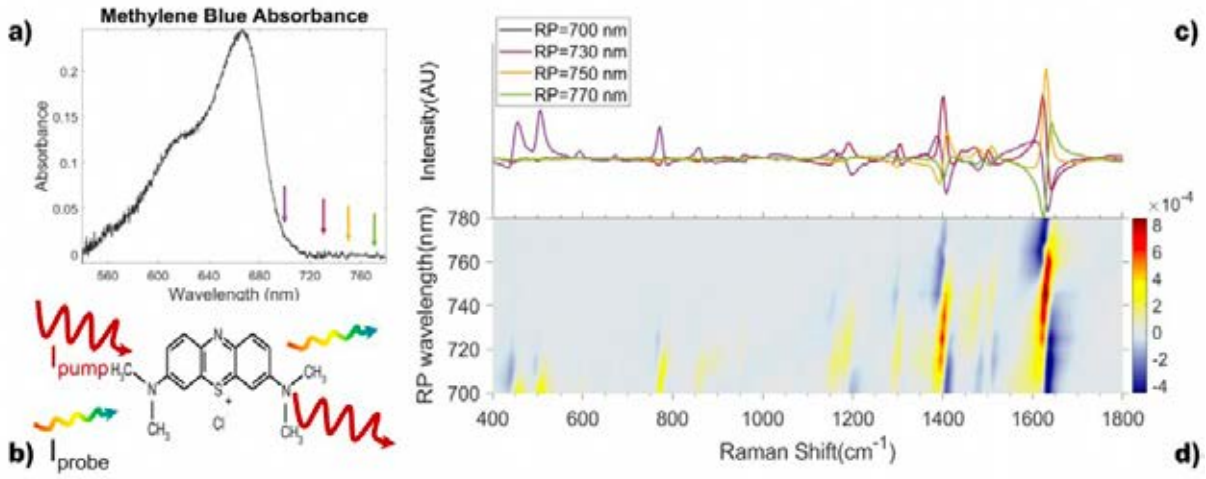
Stimulated Raman Scattering (SRS) is a robust nonlinear spectroscopic technique that overcomes the limitations of spontaneous Raman (SR) scattering by providing high intensity, fluorescence-free coherent signals. In this work, we present a comprehensive study of the SRS response of Methylene Blue, focusing on the effects of electronic resonance on Raman spectra and the resulting lineshape dependencies.

Our experimental approach employs broadband femtosecond stimulated Raman gain/loss spectroscopy [Sci. Rep. 2016, 6, 18445], which enables the coherent stimulation and heterodyne detection of diverse molecular vibrations. By tuning the excitation field into pre-resonance with Methylene Blue's electronic absorption band, the Raman cross-section is selectively enhanced. Figure 1 shows the stimulated Raman spectra acquired on the blue side of the Rama pump (RP) wavelength, providing a 2D mapping of the Raman gain as a function of the resonance condition. Notably, in contrast to standard SR spectroscopy and the SRS response (gain) on the red side, the blue-side resonance condition is detuned from the electronic absorption by a vibrational quantum. In this regime, background effects, such as RP-induced transient absorption, are significantly minimized.

Our findings demonstrate that SRS provides profound insights into both the equilibrium and excited-state properties of the system. The spectral information encoded in the complex resonant lineshapes allows us to disentangle the manifold of field interactions contributing to the third-order nonlinear response. Importantly, under specific experimental conditions, the technique facilitates the direct identification of key excited-state vibrational modes, particularly those that are Franck-Condon active. The analysis of these modes sheds light on structural dynamics and the coupling between electronic and nuclear degrees of freedom during the photoexcitation process. Overall, this study highlights the versatility of resonant SRS as a powerful structural probe for complex chromophores, successfully bridging the gap between steady-state properties and ultrafast excited-state structural evolution.

Keywords: Stimulated Raman Scattering, Methylene Blue, Resonance Raman, Excited State, Lineshape Analysis

Figure 1



a) Absorption profile of Methylene Blue in aqueous solution. The colored arrows indicate a subset of the probed Raman pump (RP) excitation wavelengths. b) Schematic representation of the SRS process on the Methylene Blue molecule. c) SRS blue-side spectra acquired at the different RP wavelengths indicated in a). d) 2D colormap of the blue-side Raman signal as a function of the Raman shift and the RP wavelength.

[Abstract:0400] [Non-linear/Time-resolved]

Controlling Electron-Phonon Coupling Via Ultrashort Core-Resonant X-Ray Pulses

Remi Claude[1], Oleg Dogadov[2], Paolo Cattaneo[1], Giovanni Batignani[3], Agata Azzolin[4], Sabine Rockenstein[4], Giulio Cerullo[5], Tullio Scopigno[3], Francesca Calegari[4], Fabrizio Carbone[1], Michele Puppin[1], Oliviero Cannelli[4]

[1]École Polytechnique Fédérale de Lausanne (EPFL), Lausanne 1015, Switzerland
[2]Fritz Haber Institute of the Max Planck Society, Berlin 14195, Germany
[3]Sapienza Università di Roma, Roma I-00185, Italy
[4]Center for Free-Electron Laser Science, DESY, Notkestraße 85, 22607 Hamburg, Germany
[5]Politecnico di Milano, I-20133 Milano, Italy

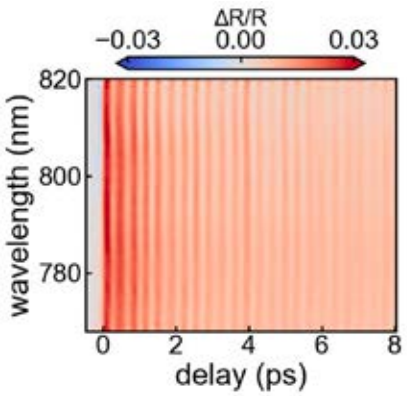
Selective control of electron-phonon coupling offers a route to drive displacive lattice dynamics and tune material functionality in condensed-matter systems. Most ultrafast studies, however, rely on near-infrared or visible excitation across the band gap, which provides limited leverage over the microscopic origin of the driving force. Here, we experimentally demonstrate displacive coherent lattice dynamics in quantum materials initiated by ultrashort extreme-ultraviolet pulses tuned in resonance with different core transitions.

In trigonal tellurium, a single-shot chirped detection scheme implemented at the FERMI free-electron laser (FEL) enables measurements of coherent phonons over a broad fluence range. Their amplitude follows the predictions of the displacive excitation of coherent phonons framework, establishing its applicability under core-resonant excitation. Ab initio calculations extend this description to include multiple band contributions and reveal how ultrafast carrier relaxation reshapes the time-dependent electron-phonon force through competing terms.

Consistently with this picture, we extend our FEL-pump/optical-probe scheme to the multielement Ta2NiSe5 system and demonstrate state-selective coherent-phonon activation by tuning the excitation pulse into resonance with different core transitions. Our study highlights how tailored electronic excitations provide a microscopic route to engineer the displacive lattice driving force with element-selective X-ray excitation.

Keywords: Electron-Phonon Coupling, Control, Quantum Materials, Coherent Phonons, Displacive Excitation

FEL-pump/optical-probe of Ta2NiSe5



Transient reflectivity map of Ta2NiSe5 obtained after core-resonant excitation and probed in the 790-820 nm spectral region. The response is dominated by a coherent oscillation involving beating of multiple phonon modes

[Abstract:0401] [Biology/Biomedicine]

From Accuracy to Interpretability: Explainable AI for Reliable Classification of Cancer Cells Using Raman Spectroscopy

***Hemanth Noothalapati*[1], *Ajinkya Deepa Deepak Anjikar*[2], *Mengxin Yang*[1], *Tatsuyuki Yamamoto*[1]**

[1]*Faculty of Life And Environmental Sciences, Shimane University, Matsue, Japan*
[2]*The United Graduate School of Agricultural Sciences, Tottori University, Tottori, Japan*

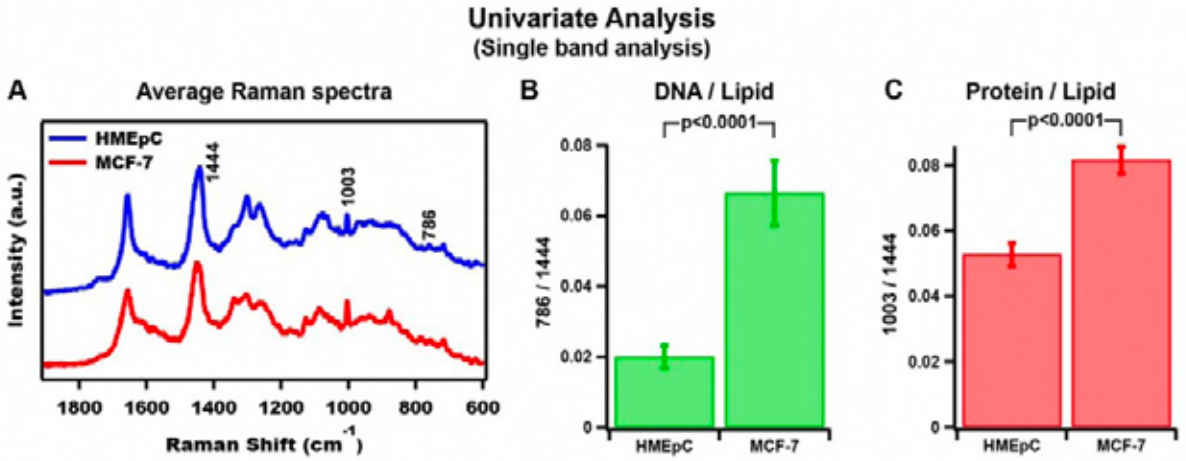
Raman microspectroscopy combined with artificial intelligence (AI) has emerged as a powerful approach for label-free, non-invasive cancer diagnostics. While modern machine learning and deep learning models achieve high classification accuracy, their lack of interpretability limits clinical translation, as decisions must be both accurate and chemically meaningful. In this work, we present a comprehensive explainable AI framework for Raman-based classification of breast cancer cells, integrating two complementary interpretability strategies: SHapley Additive exPlanations (SHAP) and a newly developed MCR-LIME approach.

Raman spectra were acquired from normal human mammary epithelial cells (HMEpC) and breast cancer cells (MCF-7) using confocal Raman microspectroscopy (Figure 1). A Feed Forward Neural Network (FFNN) was trained with augmented spectral data, achieving high classification performance. To interpret model decisions, SHAP analysis was employed to quantify the contribution of each Raman wavenumber, generating a full-spectrum "importance profile" linked to biomolecular features such as nucleic acids, proteins and lipids. To further enhance chemical interpretability, we introduce an MCR-LIME framework that combines Multivariate Curve Resolution - Alternating Least Squares (MCR-ALS) with Local Interpretable Model-agnostic Explanations (LIME). This approach enables interpretation at the level of resolved biochemical components rather than individual spectral variables, bridging the gap between statistical learning and molecular specificity. While SHAP provides global and local feature attribution across the entire spectrum, MCR-LIME offers component-level insights aligned with physically meaningful spectral signatures.

The combined framework allows systematic evaluation of whether AI models rely on chemically relevant information or spurious signals, thereby enabling feature-aware model selection beyond accuracy metrics. Additionally, the approach provides mechanistic insight into classification outcomes and reveals the influence of cellular heterogeneity on prediction behavior. This study establishes a dual-modality explainable AI strategy for Raman spectroscopy, improving both reliability and interpretability of AI-driven diagnostics. The proposed framework is generalizable to other spectroscopic datasets and represents a significant step toward clinically deployable, trustworthy AI systems in biomedical spectroscopy.

Keywords: Raman spectroscopy, Explainable AI, SHAP, MCR-ALS, LIME, Breast cancer diagnosis

Raman Spectra of normal (HMEpC) and breast cancer (MCF7) cells. (A) Average Raman spectra and (B-C) results of univariate analysis of DNA and proteins, respectively.



[Abstract:0402] [Materials]

Tracking Structural Changes in Graphene Oxide: From Established Raman Signatures to Fragmentation Effects

***Krystian Pupel*, Barbara Pałys**

Faculty of Chemistry, University of Warsaw, Warsaw, Poland

Raman spectroscopy is one of the most commonly used tools to study carbon-based materials, but interpreting spectra of highly disordered systems such as graphene oxide (GO) is still not straightforward. In our previous work, we focused on understanding how Raman features relate to structural changes in GO, particularly in terms of defects and disorder.

Building on this, we now investigate a less explored but important aspect: fragmentation of graphene oxide. When GO flakes are broken into smaller pieces, either chemically or mechanically, their structure changes significantly, especially in terms of edge density and defect distribution. These changes are expected to influence Raman spectra, but the relationship is still not fully understood.

In this work, we combine established Raman analysis with initial studies on fragmented graphene oxide. Early results show noticeable changes in the D and G bands, suggesting that fragmentation leads to more than just an increase in disorder. Instead, it appears to introduce specific structural features that can be identified spectroscopically. Our goal is to connect these observations with previous findings and move towards a more consistent interpretation of Raman spectra for graphene oxide across different structural regimes. This could help in better understanding how processing methods affect material properties and open new possibilities for controlled modification of GO.

Overall, this work shows that Raman spectroscopy can be a useful tool not only for characterizing graphene oxide, but also for tracking its transformation during fragmentation.

Keywords: graphene oxide, fragmentation, structural disorder, defects, carbon materials

[Abstract:0403] [SERS/TERS/Plasmonics]

EC-SERS Studies of Chloramphenicol on Nanostructured Gold – Control of Adsorption, Redox Transformation and SERS Signal Enhancement

***Kacper Jędrzejewski*, Barbara Pałys**

Faculty of Chemistry, University of Warsaw, Warsaw, Poland

Chloramphenicol (CAP) is a broad-spectrum antibiotic whose presence in the environment and food is strictly regulated due to its toxic and genotoxic effects. The development of sensitive detection methods and understanding of its interactions with metal surfaces are crucial for trace analysis and the design of sensing platforms. However, direct detection of CAP by SERS is challenging due to its limited affinity for noble metal surfaces, resulting in weak adsorption. In this context, electrochemical surface-enhanced Raman spectroscopy (EC-SERS) represents an attractive approach, enabling active control of analyte–surface interactions via the applied potential and modulation of the SERS response.

In this work, EC-SERS was applied to investigate the adsorption of chloramphenicol on nanostructured gold surfaces using screen-printed electrodes modified with gold nanoparticles. Raman spectra were recorded as a function of the applied potential, allowing control of interfacial conditions and monitoring of potential-dependent changes in the SERS response. An increase in signal intensity was observed upon application of electrode potential. At negative potentials, reduction of chloramphenicol occurs, accompanied by changes in spectral features, whereas at positive potentials an increase in signal intensity accompanied by spectral changes is observed, which may be related to enhanced adsorption and/or a different molecular orientation at the surface, possibly involving other functional groups interacting with the electrode. The spectroscopic results were correlated with electrochemical measurements, enabling interpretation of the observed effects in terms of redox processes and reorganization of the adsorbed layer.

Additionally, the reversibility of the system response was evaluated by examining the return of the signal to initial conditions upon reversal of the polarization direction. The results demonstrate that EC-SERS is an effective tool for investigating and controlling the interactions of chloramphenicol with metallic surfaces, providing valuable insight for the design of sensitive and selective SERS-based sensing platforms.

Keywords: EC-SERS, chloramphenicol, adsorption, gold, electrochemistry

[Abstract:0408] [Biology/Biomedicine]

High-Throughput Compressed-Sensing Raman Microscopy for Label-Free Cellular Differentiation Analysis

***Parvin Ghalebtarash*[1], *Mirte Douwes*[1], *Stefan Semrau*[2], *Thomas Schmidt*[1]**

[1]*Leiden Institute of Physics, Leiden University, Leiden, The Netherlands*
[2]*New York Stem Cell Foundation Research Institute, NY, USA*

Stem cell–based therapies and personalized medicine require noninvasive, high-efficiency quality control of cell cultures. Although Raman microscopy offers a promising label-free approach, conventional implementations are limited by slow acquisition speeds, constraining high-throughput applications. Here, we present an advanced Raman microscopy platform that integrates compressed sensing (CS) with high-resolution wide-field and confocal imaging. The system combines volume-grating based spectral separation, digital micromirror device based compression, and single-photon counting avalanche photodiode detection to enable a digitally reconfigurable spectral-fingerprint imaging modality.

To further enhance the CS framework, we introduced a Hadamard-based acquisition mode that significantly suppresses detector noise, and thus improves signal-to-noise ratio (SNR) and detection sensitivity relative to conventional spectral sampling. System characterization demonstrates a spectral resolution of ~1cm^{-1}, with lateral and axial resolution of 1 μm and 2 μm, respectively. These values correspond to a confocal volume of 3 ± 1 μm^3 and an effective detection volume of 8 ± 3 μm^3. We validate the platform's specificity by identifying multiple compounds, including guanidine hydrochloride, components of paracetamol, acetonitrile, and bovine serum albumin (BSA), across a range of concentrations. Furthermore, we demonstrate discrimination between distinct standard cell lines based on their Raman signatures. Together, these results establish the enhanced performance of our multimodal approach and highlight its potential for high-throughput, label-free cellular analysis and real-time biomolecular monitoring.

Keywords: Raman microscopy, Compressed sensing, Cell differentiation

[Abstract:0409] [Materials]

Incorporation of Nitrogen into Nanocrystalline Diamond - a Multi-Wavelength Raman Spectroscopic Study

***Miklos Veres*[1], *Laszlo Himics*[1], *Dávid Gál*[1], *Roman Holomb*[1], *Cyril Popov*[2], *Victor Ralchenko*[3]**

[1]*HUN-REN Wigner Research Centre for Physics, Budapest, Hungary*
[2]*University of Kassel, Kassel, Germany*
[3]*Prokhorov General Physics Institute of Russian Academy of Sciences, Moscow, Russia*

Nanocrystalline diamond (NCD) incorporating nitrogen at specific defect sites has unique optical emission properties, making it a very promising host material for quantum sensing, quantum bit sources, or biocompatible photoluminescent markers. NDC films contain diamond nanocrystallites (grains), an intergrain phase inbetween them and the grain boundaries separating the two. While the first constituent is a crystalline phase of sp^3 hybridized carbon atoms, the second is an amorphous carbon matrix containing a mixed network of both sp^3 and sp^2 hybridized C atoms (and hydrogen). At the grain boundaries, the ordered crystallites put constrains on the possible structural units, resulting in the formation of sp^2 carbon chains.

Raman spectroscopy is routinely used to characterize NCD, and it could give information on the bonding properties of all three constitutents. By using different Raman excitation energies specific structural units can be excited resonantly: UV excitation is suitable for the diamond crystallites, visible light for the grain boundaries and smaller structural units of the amorphous phase, while near-infrared excitation for the larger sp^2 clusters.

In this work, multi-wavelength Raman spectroscopy was used to study the incorporation of nitrogen into the different constituents of the NCD film. Series of NCD samples of different nitrogen content were characterized by using UV, visible and near-infrared excitation, and the effect of nitrogen concentration on the formed nitrogen-containing structural units was determined. The results indicate strong amorphization of the diamond structure and different routes of nitrogen incorporation into the structural units.

Keywords: Nanocrystalline diamond, nitrogen incorporation, Raman spectroscopy, multi-wavelength excitation

[Abstract:0413] [Materials]

Exploring the Length Saturation Limit of Carbon Atomic Wires by UV Resonant Raman Spectroscopy

***Marco Agozzino*[1], *Simone Melesi*[1], *Alessandro Gessini*[2], *Barbara Rossi*[2], *Valeria Russo*[1], *Carlo Spartaco Casari*[1]**

[1]*Department of Energy, Micro and Nanostructured Materials Laboratory, Politecnico di Milano, Via Lambruschini 8, Milano, 20133 Italy*
[2]*Elettra Sincrotrone Trieste, S.S. 114 km 163.5, Basovizza, 34149, Trieste, Italy*

Carbyne, the ideal one-dimensional carbon allotrope, consists of an infinite array of carbon atoms in the sp hybridisation state connected by either cumulated double bonds (cumulene, metallic) or alternating single and triple bonds (polyyne, semiconducting, favoured due to

Peierls distortion). Carbyne is expected to exhibit exceptional mechanical, electrical, and nonlinear optical properties but has up to now eluded empyrical investigation. Finite Carbon Atomic Wires (CAWs) exhibiting length and termination-dependent properties have instead been extensively studied as a model for the ideal carbyne. These peculiar characteristics arise from strong π-conjugation and electron–phonon coupling, which can be effectively probed by vibrational spectroscopy. Indeed, sp-carbon chains exhibit a collective vibrational mode named effective conjugation coordinate (ECC) that falls in the usually silent 1800–2300 cm−1 spectral region. The ECC mode is highly sensitive to conjugation, providing direct insight into the electronic structure of CAWs.

However, the low concentration of CAWs achievable in solution hinders their investigation by conventional Raman spectroscopy. This limitation can be overcome by tuning the excitation wavelength to match their vibronic absorptions, greatly enhancing the signal through resonant Raman scattering.

In this work, we present a detailed vibrational study of polyynic CAWs with hydrogen, halogen, and organometallic terminations, with chain lengths up to 24 carbon atoms. UV resonant Raman spectroscopy with a tunable laser source in the range between 191-315 nm and 350-475 nm allows detection of the ECC mode and its overtones up to the eighth order. This enables reliable quantification of the length-dependent Raman cross section and the evolution of vibrational anharmonicity. Notably, the anharmonicity shows a linear dependence on bond length alternation (BLA), consistent with previous studies on short hydrogen-terminated chains and nanotube-confined systems. This finding indicates that anharmonicity is a universal property of carbyne-like materials, governed solely by BLA, and provides new input for modeling the length-dependent properties of CAWs toward the carbyne limit.

Keywords: Carbon Atomic Wires, Carbyne, Resonant Raman, Anharmonicity

[Abstract:0414] [Non-linear/Time-resolved]

Harnessing the Coupling of Photocarriers to Lattice Displacements in Low Dimensional Perovskites: an İmpulsive Vibrational Spectroscopy Perspective

Emanuele Mai[1], Leonardo Marsano[2], Neethish Madathiparambil Mohanan[1], Ruggero Sala[2], Giovanni Batignani[1], Giulia Grancini[2], Tullio Scopigno[1]

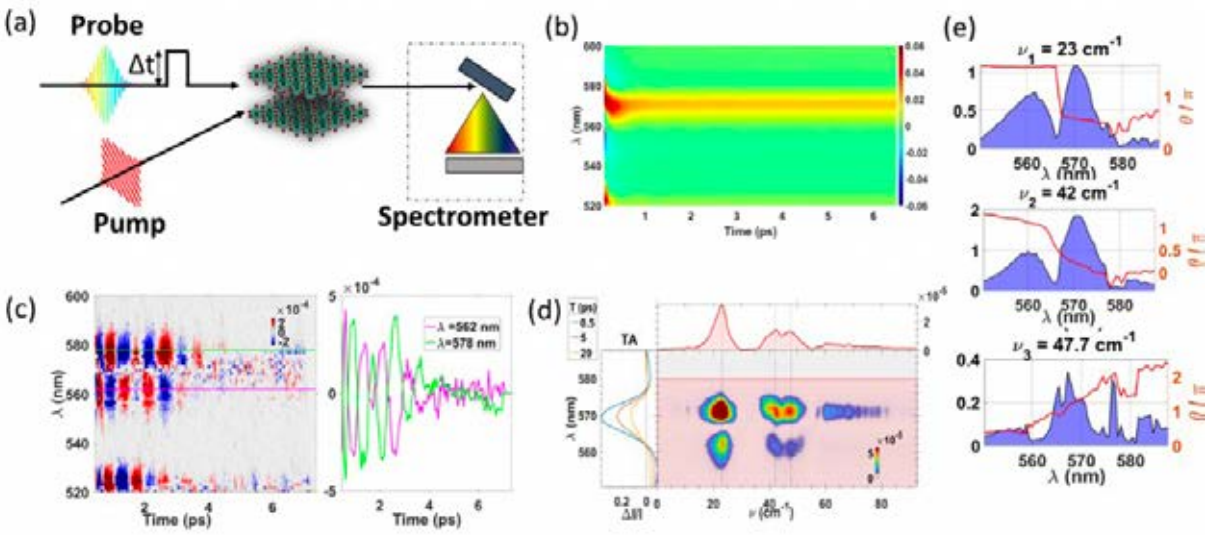
[1]Dipartimento di Fisica, Universitá di Roma "La Sapienza", Roma I-00185, Italy
[2]Department of Chemistry & INSTM, University of Pavia, Via T. Taramelli 14, 27100 Pavia, Italy.

Low-dimensional perovskites (LDPs) are attracting considerable attention due to their tunable electrical and optical properties, yet controlling their crystal growth and understanding their intrinsic charge transport mechanisms remain a hot topic of research, especially for wide bandgap low-n LDPs. Recently, it has been demonstrated that partial substitution of iodine with chlorine at the equatorial position induces vertical crystal growth, overcoming transport limits and yielding record power conversion efficiencies [*Nat. Commun. 2024, 15, 9069*].

A fundamental aspect governing the optoelectronic behaviour of these highly efficient materials is the interaction between electronic properties and lattice vibrations, which are strongly correlated due to the soft, fluctuating nature of the perovskite crystal lattice. To explore the key role of low-frequency phonons in determining the carrier dynamics and unravel ultrafast electron-phonon couplings, we performed Impulsive Vibrational Spectroscopy (IVS) [*Nat. Commun. 2018, 9, 1971*] experiments on LDPs. IVS provides the chance to coherently stimulate and track the nuclear motions following ultrafast photoexcitation. Operating in the time-domain, IVS also circumvents the elastic scattering limitations that typically plague low-frequency measurements, enabling the unhindered detection of these crucial soft modes. By collecting the resonant IVS response (i.e. injecting photocarriers by an ultrashort pump pulse), our measurements reveal the temporal evolution of specific low-frequency phonons, directly highlighting the structural reorganization and electron-phonon coupling effects that follow photo-carrier generation. Crucially, through time-domain phase analysis, we determine the specific phonons responsible for the structural rearrangement via a displacive excitation mechanism. Our measurements isolate the phonons most strongly coupled with the electrons, identifying reorganization energies and decoherence times as function of the crystal growth direction. The results provide a direct atomic-level perspective on the photo-induced structural distortions, offering crucial insights for the rational design of highly efficient wide band gap perovskite solar cells and related optoelectronic technologies.

Keywords: Impulsive Vibrational Spectroscopy, Low-Dimensional Perovskites, Electron-Phonon Coupling, Structural Reorganization, Photo-Carrier Generation

Figure 1



(a)Experimental scheme of Impulsive Vibrational Spectroscopy (b)Experimentally measured differential transmittance (c)Oscillatory components extracted by subtracting the Transient absorption from figure (b). (d) Fourier transformed colormap on the bottom panel, Transient Absoption at three different instants on the left panel and the integrated spectra on the top panel. (e)Fitted amplitude and Phase of different modes.

[Abstract:0417] [SERS/TERS/Plasmonics]

Rapid Inkjet Fabrication of Modular Plasmonic Chemosensors

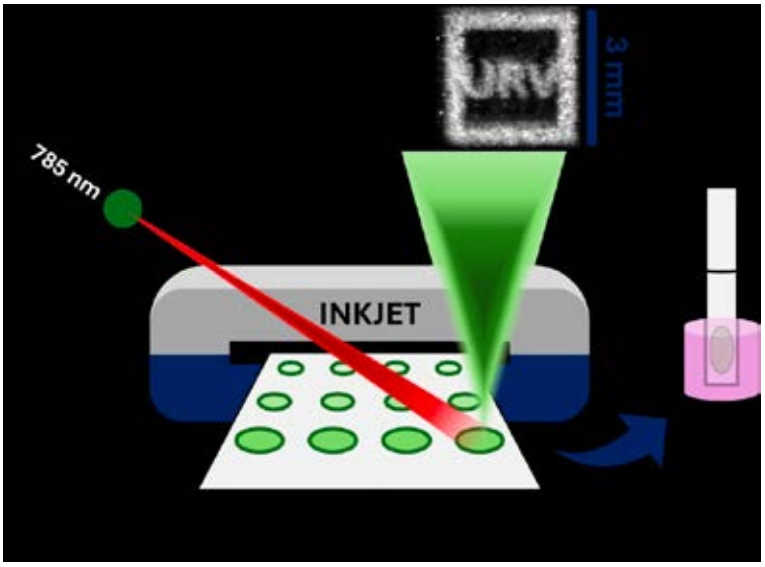
***Irving Brian Becerril Castro*[1], *Matz Liebel*[2], *Ramón Alvarez Puebla*[3]**

[1]*Department of Physical and Inorganic Chemistry, Universitat Rovira i Virgili, Spain*
[2]*Department of Physics and Astronomy, Vrije Universiteit Amsterdam, The Netherlands*
[3]*Institucio Catalana de Recerca i Estudis Avancats, ICREA, Spain*

In this work, we present a novel approach to produce modular inkjet-printable surface enhanced Raman scattering (SERS) chemosensors (Figure 1). By producing plasmonic inks with functionalized metal nanoparticles, we successfully printed spatially confined, organized sensing patterns onto flexible substrates like paper. These modular sensors were coupled with a large field-of-view (9 mm^2) imaging system for a fast imaging of the chemical properties of the sample. To demonstrate the performance of these materials we print pH sensors on filter paper and used them to interrogate different pH aqueous solutions. Our results show that the sensors maintain high signal-to-noise ratios and represent a forward step towards the mass-production of on-demand SERS sensors which are readily read out via SERS imaging.

Keywords: widefield SERS, chemosensors, inkjet printing

Figure 1.



Scheme of the inkjet fabrication of modular plasmonic chemosensors

Oral Abstracts

[Abstract:0421] [Biology/Biomedicine]

Detection of Single Nucleotide Variants Using Alkyne-Tagged Raman-Active DNA Probes

***Roman Holomb*[1], *Huy Van Nguyen*[2], *John S. Fossey*[2], *James H.R. Tucker*[2], *László Himics*[1], *Tamás Váczi*[1], *Attila Csáki*[1], *Miklós Veres*[1]**

[1]*Institute for Solid State Physics and Optics, HUN-REN Wigner Research Centre for Physics, Budapest, Hungary*
[2]*School of Chemistry, University of Birmingham, Birmingham, UK*

Single nucleotide variants (SNVs) are critical biomarkers in numerous diseases, including cancer. Yet their accurate detection at single-base resolution remains challenging, particularly for imaging-based approaches requiring non-fluorescent readout strategies. Here, we introduce a Raman spectroscopy-based method for sequence-specific detection of nucleobases in DNA using alkyne-tagged oligonucleotide probes.

Ab initio calculations predicted that the alkyne stretching vibration of 5-ethynyluracil is highly sensitive to hydrogen-bonding interactions with complementary nucleobases. This effect was experimentally validated by incorporating 5-ethynyl-2′-deoxyuridine into synthetic DNA probes and monitoring Raman spectra in the bio-orthogonal silent region (2000 – 2400 cm-1). Upon DNA hybridization, distinct and reproducible shifts in the alkyne Raman band were observed, enabling direct detection of base pairing. Furthermore, mismatched base pairs produced larger and characteristic frequency shifts compared to fully matched duplexes, allowing discrimination between all four canonical nucleobases (A, T, C and G) at a single position. This capability was further demonstrated through the detection of a clinically relevant mutation (BRAF V600E), where the mutant and wild-type sequences exhibited clearly distinguishable Raman signatures. Therefore, the method shows high specificity and reproducibility, with signal-to-noise ratios sufficient for reliable peak position determination. The Raman response was found to be highly localized, enabling site-specific detection of SNVs only when the alkyne tag is positioned adjacent to the target base. Unlike fluorescence-based probes, this approach benefits from narrow spectral features, minimal background interference, and compatibility with multiplexing through bio-orthogonal vibrational tags.

This work establishes a new Raman-based readout mechanism for nucleic acid hybridization that directly probes hydrogen-bonding interactions via vibrational frequency shifts. While current sensitivity is limited by spontaneous Raman scattering, integration with signal enhancement strategies such as surface-enhanced Raman spectroscopy (SERS) and nucleic acid amplification methods offers a clear pathway toward practical diagnostic applications. The approach provides a foundation for future developments in Raman-based biosensing and imaging of genetic variations in complex biological systems.

Keywords: Raman spectroscopy, ab initio calculations, single nucleotide variants, DNA hybridization, alkyne tagging

[Abstract:0423] [SERS/TERS/Plasmonics]

Time-Lapse Metabolic Fingerprinting of Bacterial Stress Responses Using Surface-Enhanced Raman Spectroscopy

***Markéta Benešova*[1], *Silvie Bernatova*[1], *Marc Lamy de la Chapelle*[2], *Mathieu Edely*[2], *Jan Jezek*[1], *Martin Kizovský*[1], *Ota Samek*[1]**

[1]*Institute of Scientific Instruments of the CAS, v. v. i., Brno, Czech Republic*
[2]*Le Mans Université, Le Mans, France*

Rapid and accurate detection of bacterial physiological states, such as viability and stress responses, is essential for microbiology research and clinical diagnostics. Conventional culture-based methods are often slow, potentially delaying targeted medical therapy, while traditional molecular approaches may fail to capture dynamic metabolic changes. Surface-enhanced Raman spectroscopy (SERS) offers a powerful, non-invasive alternative for rapid characterization of microorganisms in real-time and time-lapse (long-term) measurements.

By applying bacterial culture directly onto SERS active structures, the biochemical composition of the cell surface or external metabolites released by the bacteria can be analyzed and detected. Thus, SERS has been successfully used in our lab to observe bacterial responses to various stressors, including osmotic stress or antibiotic treatment.

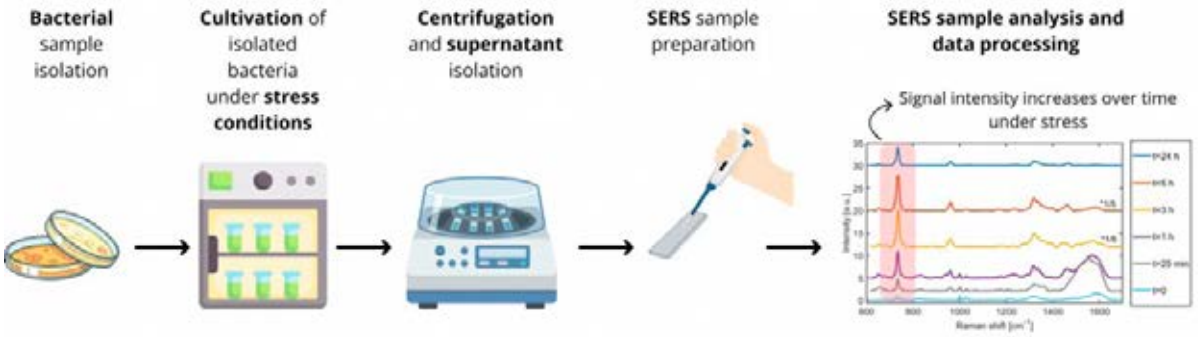
Here we present that under stress conditions, bacteria secrete specific purine-based metabolites (notably adenine specific for *Staphylococcus aureus*; and adenine and hypoxanthine specific for *Escherichia coli*), which function as sensitive biomarkers for bacterial physiological states.

Metabolites such as adenine immediately accumulate near bacterial cells, making them optimal SERS target molecules. Their release, recorded in time-lapse experiments (up to 24 hours), reflects the purine-salvage pathways, providing a phenotypic stress reflection to external stress, such as antibiotic exposure or environmental shifts (Figure 1). Consequently, time-lapse SERS can provide a novel probe to further our understanding of microbial metabolism and dynamic features in microbial biology.

Acknowledgment: This work was supported by the Czech Academy of Sciences, grant number (CNRS-26-08, "*Raman spectroscopy for characterization of metabolites secreted from bacteria*").

Keywords: SERS, Real-time SERS, Time-lapse SERS, Bacterial stress response

Figure 1: The SERS measurement of the {Staphylococcus aureus} using a gold substrate to enhance the signal of the external metabolites, here exemplified for adenine (highlighted spectra on the right side of the picture).



The figure should be placed after the main text, before the Acknowledgment section.

Oral Abstracts

[Abstract:0424] [Biology/Biomedicine]

Decoding Drug Response Across Systems: Raman Insights from Endothelium to Leukemia

***Katarzyna Majzner*[1], *Patrycja Dawiec*[2], *Jagoda Orleańska*[3]**

[1]*Department of Chemical Physics, Faculty of Chemistry, Jagiellonian University, Gronostajowa 2, 30-387 Krakow, Polan*
[2]*Doctoral School of Exact and Natural Sciences, Jagiellonian University, Łojasiewicza 11, 30-348 Krakow, Poland*
[3]*Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, Krakow 31-342, Poland*

Targeted therapies have advanced leukemia treatment, improving outcomes by modulating molecular pathways vital for cancer cells. They use compounds such as inhibitors to interfere with signaling pathways. Despite success, resistance, off-target effects, and adverse reactions can limit long-term effectiveness, highlighting the need to better understand cellular responses to therapy.

Resistance to targeted therapies is a complex, multifactorial phenomenon involving dynamic metabolic reprogramming. Our research on endothelial cells treated with tyrosine kinase inhibitors (TKIs) showed that therapies cause biochemical disturbances, including oxidative stress, mitochondrial dysfunction, and lipid remodeling, as observed by Raman and fluorescence imaging. [1] These findings show targeted drugs cause broad metabolic adaptations, supporting the idea that cellular response to therapy depends more on biochemical phenotype than genetic background.

Raman spectroscopy is a powerful tool for analyzing cellular biochemistry, revealing molecular changes linked to drug response. It produces a spectral fingerprint of lipids, proteins, nucleic acids, and metabolites, allowing study of phenotypic heterogeneity in hematological malignancies. [2,3] Previous studies show it can differentiate normal from malignant cells and detect subtle biochemical differences related to various cellular states. [2,3] Importantly, this technique enables monitoring cell–drug interactions and early markers of therapeutic response.

In this study, we use Raman imaging, along with biochemical assays, to examine molecular and metabolic changes in leukemia cells exposed to targeted therapies. Our approach focuses on identifying spectral signatures associated with drug response. By capturing phenotypic diversity and linking it to treatment outcomes, we aim to create a robust, label-free pipeline to monitor therapy effectiveness and uncover resistance mechanisms. This approach could eventually support developing more effective, personalized treatments leukemia.

Acknowledgement: This research was partially funded by the National Science Center Poland (NCN), PRELUDIUM 23 UMO-2024/53/N/ST4/03000. The research has been supported by a grant from the Faculty of Chemistry under the Strategic Programme Excellence Initiative at Jagiellonian University. KM acknowledges the support received as a fellow of the *L'Oréal-UNESCO For Women in Science* Programme.

References:

[1] J. Orleanska et al., Analyst, 2025, 150, 527-547

[2] P. Dawiec et al., SAA, 309 (2024).

[3] P. Leszczenko et al., Analyst, 2024, 149, 5443-5454

Keywords: Raman Spectroscopy, Targeted therapies, Leukemia, Endothelium, Chemometrics

Oral Abstracts

[Abstract:0426] [SERS/TERS/Plasmonics]

Lock-in Sampling: a Time-Domain Strategy for High-Speed Widefield SERS Imaging

***Ting Wang*[1], *Irving Brian Becerril Castro*[2], *Ramon Alvarez Puebla*[3], *Matz Liebel*[1]**

[1]*Department of Physics and Astronomy, Vrije Universiteit Amsterdam, De Boelelaan 1100, Amsterdam 1081 HZ, The Netherlands*
[2]*Department of Physical and Inorganic Chemistry, Universitat Rovira i Virgili, Carrer de Marcel·lí Domingo 2-4-6, 43007, Tarragona, Spain*

Surface-enhanced Raman spectroscopy (SERS) enables non-destructive, multiplexed measurements with high molecular specificity and single-molecule sensitivity. Despite these attributes, the most widely adopted readout approach for SERS spectra, confocal Raman systems performing serial raster scanning, leaves many of these advantages untapped, particularly in terms of throughput, nanoscale imaging, and spectral multiplexing. This has impeded both the scientific advancement and commercialization of the technology. Fourier-transform imaging offers a compelling alternative by operating in the time rather than the frequency domain, enabling simultaneous full-spectrum acquisition at every camera pixel. However, high spectral quality comes at the cost of collecting thousands of images, severely limiting acquisition speed. Here we present lock-in sampling, a time-domain acquisition strategy that achieves spectral quality on par with conventional Fourier-transform methods while requiring for only a few hundred images at near-random sampling. The key insight is that the relatively narrow Raman spectral range of interest (~1500 cm^{-1}) allows large sampling step sizes far exceeding those of conventional approaches based on Nyquist-Shannon sampling theorem, preserving spectral resolution while dramatically shortening acquisition times. A dedicated reference channel tracks the path-length difference, or time-delay, between the interferometer arms, enabling accurate spectral reconstruction even from irregularly sampled interferograms. We benchmark lock-in sampling against conventional Fourier-transform acquisition, confirming comparable spectral quality, before imaging thousands of individually resolved, multiplexed SERS amplifiers at readout speeds orders of magnitude faster than existing methods. Experiments on multiplexed 3D volumetric samples, spanning randomly mixed and spatially structured configurations, demonstrate reliable identification and imaging throughout. Taken together, these results establish lock-in sampling as a general and versatile framework with broad potential across Raman, SERS, and any Fourier-like acquisition scheme.

Keywords: SERS imaging, Fourier-transform spectroscopy, lock-in sampling, non-uniform sampling

[Abstract:0427] [Novel Approaches]

Alternative Application of Time-Gated Raman Spectrometer: Leveraging Picosecond Time-Gating for Fluorescence Lifetime Sensing of Molecular Diffusion in Collagen Hydrogels

***Jacopo Zini*[1], *Shirin Tavakoli*[1], *Natasha Zashikhina*[2], *Iuliia Pilipenko*[2], *Timo Laaksonen*[1], *Michael Gertz*[3], *Antonello Caruso*[3], *Arto Urtti*[2]**

[1]*University of Helsinki, Faculty of Pharmacy, Division of Pharmaceutical Biosciences, Helsinki, Finland*
[2]*School of Pharmacy, University of Eastern Finland, Kuopio, Finland*
[3]*Pharmaceutical Sciences, Roche Innovation Center Basel, Roche Pharma Research and Early Development, Basel, Switzerland*

Quantifying the diffusion coefficient (D) of molecules within hydrogel matrices, such as collagen, is essential for predicting drug delivery efficacy. Traditional methods for measuring D often lack the necessary combination of being non-destructive, operator-independent, and suitable for in-line monitoring. Raman Spectroscopy (RS) presents a potential in-line alternative capable of assessing both molecular concentration and hydrogel integrity. However, its application is frequently hindered by a high Limit of Quantification (LoQ).

To address these limitations, we employed Time-Gated Raman Spectroscopy (TG-RS) in conjunction with fluorescently labeled molecules. While traditional RS relies on time-integrating sensors that capture Raman and fluorescence photons simultaneously, often resulting in signal masking, TG-RS utilizes CMOS Single-Photon Avalanche Diodes (SPADs) and Time-to-Digital Converters (TDCs) to achieve picosecond temporal resolution. This architecture allows the system to "time-label" photons, discriminating between early Raman scattering and late fluorescence emission.

In this study, the fluorescence intensity, which remains too high to resolve the Raman signal, was used to determine the D, while the picosecond temporal resolution of the TG-RS system enabled the determination of the fluorescence lifetime (τ) of the molecular labels. This lifetime measurement served as a robust proxy for hydrogel integrity and viscosity. By simultaneously measuring fluorescence intensity (to determine D) and fluorescence lifetime (to monitor hydrogel stability), we were effectively able to measure the D of protein – bovine serum albumin (BSA) – in a natural hydrogel and simultaneously assess the integrity of the hydrogel. The experimental D value (78.46 ± 27 μm2/sec) for BSA was comparable with the calculated D (87.07 μm2/sec) using Stoke-Einstein equation at 35 °C.

This work redefines the utility of TG-RS instrumentation by demonstrating that the high temporal resolution required for fluorescence suppression can be repurposed for fluorescence lifetime sensing. Additionally, our results indicate that TG-RS instrumentation provides a comprehensive characterization of drug dynamics even when Raman scattering is completely suppressed.

Keywords: Time Resolved, Time-Gated, Fluorescence Lifetime, Molecular Diffusion, drug development

[Abstract:0430] [Biology/Biomedicine]

Unlocking the Wound-Healing Potential of Tarantula Cubensis Venom: Migration, Cytotoxicity, and Raman Spectroscopic Profiling in a Human Dermal Fibroblast Model

***Nihal Simsek Ozek*[1], Ferhunde Aysin[1], Irfan Sefiloğlu[2], Irem Alparslan[2], Mustafa Akay[2]**

[1]East Anatolia High Technology Application and Research Center (DAYTAM), Atatürk University, Erzurum, Türkiye,Department of Biology, Faculty of Science, Atatürk University, Erzurum, Türkiye.
[2]Remzi Sakaoğlu Science and Art Center, Erzurum, Türkiye.

Decubitus ulcers are chronic wounds that occur due to pressure and are associated with considerable morbidity and reduced quality of life. Natural toxins have been found to hold considerable therapeutic value in the healing of wounds. Tarantula cubensis venom, also known as "Theranekron," is an alcoholic extract used in veterinary medicine and has been found to possess anti-inflammatory and apoptotic effects. However, the wound-healing effects of this toxin have not been studied.

Therefore, this study was conducted to examine the cytotoxic and regenerative potential of Theranekron against human dermal fibroblast cells in an in vitro system and the corresponding biochemical changes using Raman spectroscopy. HDF cells treated with different concentrations of Theranekron (200-600 µg/mL) were subjected to an MTT assay to assess cytotoxicity, and IC50 values were calculated by one-way ANOVA. The scratch wound healing assay was performed with subcytotoxic concentrations (300, 350, and 400 µg/mL), and the wound area was analyzed using ImageJ software at 0, 24, 48, and 72 hours. Raman spectroscopy was done with HDF cells treated with 300 µg/mL of Theranekron and negative controls. Chemometric methods, PCA, and HCA were performed on Raman data.

The MTT assay showed that 300 µg/mL of extract maintained cell viability with high metabolic activity, with an IC50 of 500 µg/mL. A significant dose-response effect of cytotoxicity was also noted from 250 µg/mL and above ($p < 0.001$). In the scratch assay, 300 µg/mL showed maximum wound closure after 72 hours, with only 2.76% of the wound area remaining. In FTIR analysis, PCA and HCA were used to differentiate between venom and control groups, accounting for 98% of the variance. In addition, significant spectral differences were noted in the lipid, protein region and nucleic acids.

The results clearly indicate that T. cubensis venom facilitates fibroblast migration and tissue regeneration and causes detectable biochemical changes that can be measured by Raman spectroscopy. The study emphasized the efficacy of Raman spectroscopy in detecting changes in the presence of bioactive compounds and the possible application of T. cubensis venom in the development of regenerative wound healing agents.

Keywords: Spider venom, wound healing, human dermal fibroblast, Raman spectroscopy.

Oral Abstracts

[Abstract:0431] [Novel Approaches]

Asynchronous Ultrafast Spontaneous Raman Sensing

***Hankun Yang*[1], *Raouf Amara*[1], *Raj Pandya*[2], *Hilton Barbosa de Aguiar*[1]**

[1]*Laboratoire Kastler Brossel, Paris, France*
[2]*Department of Chemistry, University of Warwick, Coventry CV4 7AL, United Kingdom*

Spontaneous Raman microscopy is a powerful tool for structural characterization, yet its application to ultrafast transient phenomena is historically hindered by weak signal intensities and the slow acquisition speeds of conventional detectors. While traditional pump-probe techniques offer high temporal resolution, they require complex optical synchronization and high-peak-power pulsed lasers.

Here, we present an asynchronous ultrafast spontaneous Raman sensing method designed to probe transient dynamics in solid-state materials with nanosecond resolution. Our approach utilizes a continuous-wave (CW) excitation source and an electrical time-clock to decouple the detection window from the excitation trigger. The system employs a digital micromirror device (DMD) for high-speed spectral region selection, coupled with a single-photon avalanche diode (SPAD) and a high-precision time-tagger. By recording the arrival times of individual Raman photons relative to an external excitation signal, we reconstruct the material's temporal evolution without the need for optical delay lines.

We benchmark this technique by monitoring the insulator-to-metal transition (IMT) in vanadium dioxide (VO2). The method successfully captured both electrically and optically induced phase transitions, including the spatial propagation of the metallic phase. Notably, our results reveal a clear temporal separation between photoinduced and thermally induced transition mechanisms. This work demonstrates that asynchronous time-stamping Raman sensing provides a versatile, cost-effective alternative for investigating structural ultrafast dynamics in transient chemical and physical processes.

Keywords: Spontaneous Raman spectroscopy, Time-resolved Raman, Transient dynamics, Solid-State Materials

[Abstract:0433] [Industrial/Societal Applications]

Real-Time Raman Detection and Quantification of Molecular Gases at Ppm Level Using Hollow-Core Fiber Sensors

Sofia Julve Gonzalez[1], Iván Reyes Rodriguez[2], Marco Veneranda[2], Jose Antonio Manrique[2], Maria Mayoral[2], Lidia Asenjo[2], Sergio Jiménez[2], Aurelio Sanz Arranz[2], Guillermo Lopez Reyes[2]

[1]AstraSpec S.L. and Research Group ERICA (University of Valladolid), Boecillo, Spain
[2]Research Group ERICA and LaDIS, University of Valladolid, Spain

Accurate gas detection is of major interest for industrial safety, process control, and the transition toward cleaner energy sources. However, Raman spectroscopy in the gas phase has traditionally been limited by the low molecular density of gases and the inherently weak Raman scattering cross section, which result in faint signals and make real-time quantification challenging. Overcoming these limitations is essential for extending Raman spectroscopy toward continuous, multi-species gas monitoring under realistic operating conditions.

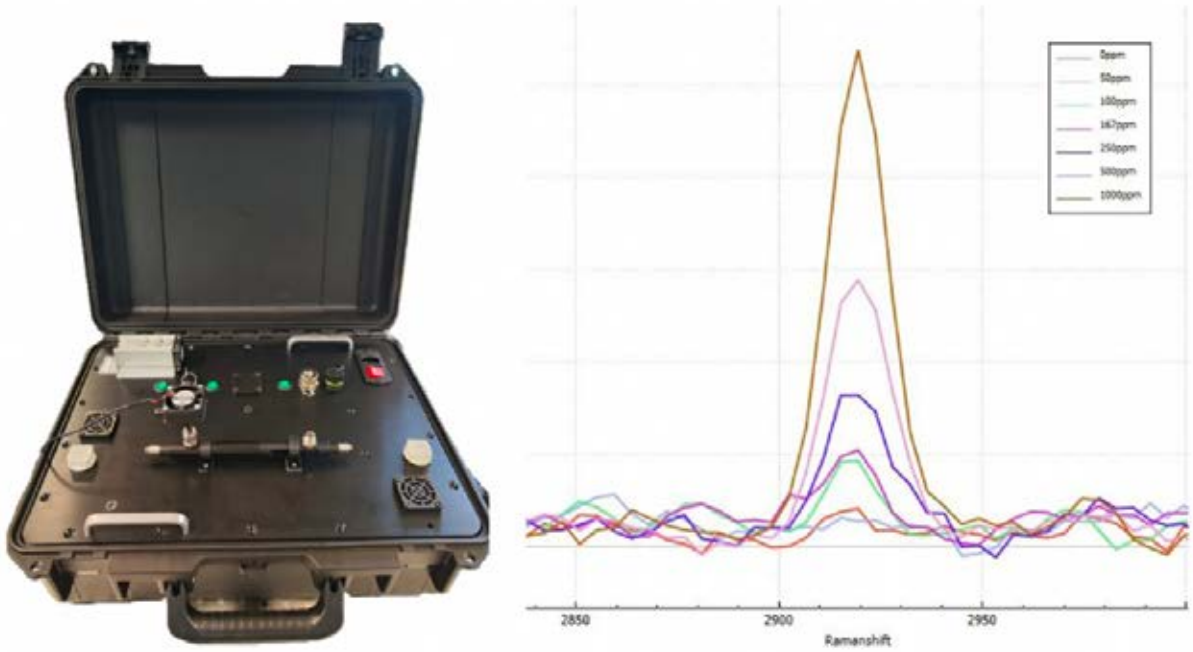
This contribution presents a Raman-based solution for the real-time detection and quantification of molecular gases at concentrations in the ppm range. The system is based on an optimized hollow-core fiber (HCF) sensor. In this approach, both the excitation laser and the gas sample are confined along the same optical path, significantly enhancing light–matter interaction and improving the sensitivity of the Raman measurement.

The sensor has been validated under controlled conditions and has shown survivability and/or reliable performance in demanding environments, including variations in pressure (vacuum to 3 bars), temperature (from criogenic to ~100ºC), and humidity (0-100% RH). This technology is of particular relevance for industrial monitoring (e.g. biogas or H2 economies), as it has been tested to measure gases such as O2, H2, H2O (liquid and vapor), CO2, CH4, H2, NOx, SOx, and NH3, among others. On this basis, dedicated calibration and multivariate data-analysis strategies are being implemented to enable simultaneous multi-gas monitoring and quantitative real-time retrieval, reaching limits of detection in the ppm range. For example, CH4 showed measurable Raman signals obtained down to concentrations of 2 ppm.

These results highlight the potential of the system for sustainable industrial applications, including biogas monitoring, hydrogen technologies, emissions control, and decarbonization processes. This work shows how Raman spectroscopy, when combined with optimized HCF architectures and quantitative analysis workflows, can evolve into a practical tool for continuous molecular gas sensing in realistic industrial scenarios.

Keywords: Raman spectroscopy, gas detection, real-time gas monitoring, biogas, hydrogen economy

Raman-based sensor setup for gas detection (left). Example of detection of CH4 for different concentrations (right).



The figure shows the Raman-based sensor setup for gas detection and analysis, as well as the detection of the CH4 band at 2920 cm-1 for different concentrations, showing detection capabilities below 100 ppm.

[Abstract:0435] [Novel Approaches]

Raman Microspectroscopy Online Coupled with Field-Flow Fractionation for Analysis of Nanoplastic Particles: From Water to Milk Matrices

***Natalia Ivleva*[1], *Stefano Giordani*[2], *Maximilian J. Huber*[1], *Valentina Marassi*[2]**

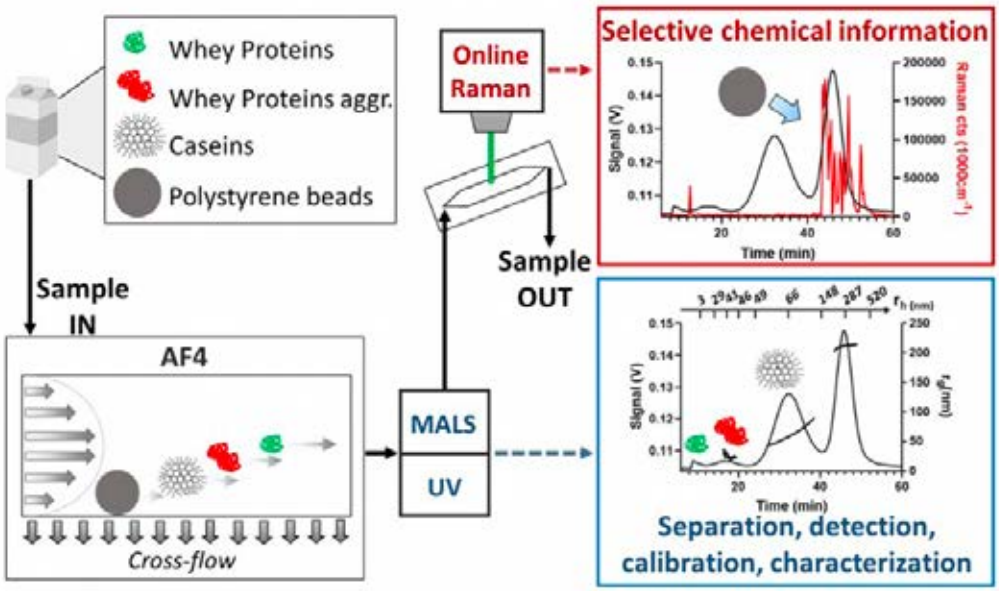
[1]*Chair of Analytical Chemistry and Water Chemistry, School of Natural Sciences, Technical University of Munich*
[2]*Department of Chemistry, University of Bologna*

Nanoplastics (NPLs, smaller than 1 μm) represent an emerging topic of relevance to environmental and food science as well as to human toxicology. NPLs are expected to have negative eco-toxicological impacts, since these tiny particles may penetrate through cell membranes. This underlines the necessity for development, optimization and validation of methods suitable for the analysis of NPLs. Here, field-flow fractionation (FFF), supported by multidetector (MD, i.e. UV and multi-angle light scattering, MALS) platform can be efficiently applied for fractionation and characterization of particle sizes. However, for chemical identification and hence a distinction between NPLs and non-plastic particles additional technique is required. This task can be performed by Raman microspectroscopy (RM), which provides characteristic fingerprint spectra and (due to its insensitivity to water) is applicable for wet samples/ suspensions.

In this presentation, the online coupling of FFF to RM for size-resolved chemical characterization of NPLs in different matrices will be discussed. To implement this hyphenation, we solve the common limitation of weak Raman signal from particles in diluted suspensions by employing an optical tweezer-based particle retention in a flow-cell. The developed setup was first tested using aqueous suspensions of mono- and polydisperse NPLs (PS, PE, PMMA) and non-plastic particles (SiO_2, TiO_2, iron oxides) in the size range of 100 nm – 5 μm. The online coupling was realized for both asymmetric flow FFF (AF4, suitable for size-based separation of particles in the size range of 1 nm – 1 μm) and centrifugal FFF (CF3, suitable for size- and density-based separation of particles in the size range of 10 nm – 50 μm) together with UV and MALS detectors – thereby providing physical characterization via MALS detector and chemical identification via RM. Next, we showed the applicability of online FFF-RM for the analysis of NPLs in a real food matrix – milk, including separation, selective detection, and multiparametric characterization of milk components and NPLs (PS beads, 100 – 500 nm) without sample pretreatment (Figure). The results were confirmed by offline analysis of the collected fraction with orthogonal techniques (SEM-EDX and nanoparticle tracking analysis, NTA), strengthening the potential of the presented approach (doi.org/10.1021/acs.analchem.5c05137).

Keywords: Nanoplastics, Fractionation, Identification, Raman

Online FFF-Raman coupling for analysis of nanoplastics in milk.



[Abstract:0437] [Novel Approaches]

Monitoring Pharmaceutical Isolation Processes through Spatially Offset Raman Spectroscopy: Dilution- and Displacement-driven Filtration-washing

***Samuel Brito Ferreira Santos*[1], *Chris J. Price*[2], *Jan Sefcik*[2], *Yi-Chieh Chen*[1]**

[1]*Department of Chemical and Process Engineering, University of Strathclyde, Glasgow, UK*
[2]*ESPRC Centre for Continuous Manufacturing and Advanced Crystallisation, University of Strathclyde, Glasgow, UK*

Washing is a fundamental isolation process in pharmaceutical manufacturing, used to replace impurity-containing crystallisation mother liquor with a clean wash solvent, thereby improving the processability of the active pharmaceutical ingredient (API) in the subsequent drying stage and contributing to final product quality. However, this process is governed by complex, not fully understood dynamics that contribute to process variability, which could alter the API's morphology and the cake's structure, and create non-uniform impurity distributions within the solid bed. These structural and spatial heterogeneities pose significant challenges in determining the endpoint of washing, leading to excessive solvent use. Although Raman spectroscopy provides chemical specificity for in-line monitoring, backscattering configurations are limited to surface probing. This study utilises a recently developed Spatially Offset Raman Spectroscopy (SORS) probe to investigate subsurface analysis of non-homogeneous systems under two washing scenarios: dilution and displacement. The model system comprised paracetamol as the API, with anisole as the initial solvent, intended to be replaced by methyl tert-butyl ether. Partial least squares regression analysis is performed to evaluate the performance of various SORS configurations and the conventional backscattering configuration on estimating residual anisole in the wet cake. Model performance improves across all configurations with the application of spectral pre-processing, which mitigates spectral variation unrelated to solvent composition. Furthermore, anisole prediction errors reduction of up to 49% are observed with models built using the SORS spectra, compared to those from the backscattering configuration, with further improvement in estimation error achieved by using standard normal variate pre-processing. This work demonstrates the capability of SORS as a technique for representative in-line analysis of non-uniform systems, supporting crucial process understanding for process efficiency and waste reduction.

Keywords: Process Analytical Technology (PAT), Solvent Monitoring, Pharmaceutical Manufacturing

[Abstract:0441] [SERS/TERS/Plasmonics]

Low-Cost, Scalable SERS Substrates Based on Copper-Assisted Chemically Etched Silicon with Inverted Surface Architectures

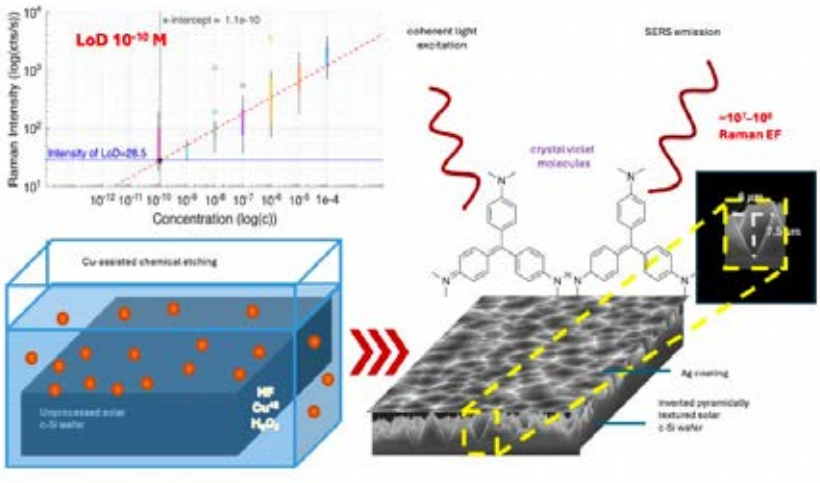
***Sinan Genc*[1], *Büşra Altınsoy*[3], *Zeynep Cantürk*[2], *Hisham Nasser*[4], *Rasit Turan*[4], *Alpan Bek*[2]**

[1]*Department of Electrical and Electronics Engineering, Abdullah Gül University, Kayseri, Turkey*
[2]*Department of Physics, Middle East Technical University, Turkey*
[3]*Department of Micro and Nanotechnology, Middle East Technical University, Ankara, Turkey*
[4]*ODTÜ-GÜNAM, The Center for Solar Energy and Applications, Middle East Technical University, Ankara, Turkey*

We present a scalable and cost-effective strategy for fabricating surface-enhanced Raman spectroscopy (SERS) substrates based on copper-assisted chemical etching (Cu-ACE) of monocrystalline silicon followed by silver coating. By systematically tuning the Cu^{2+} and H_2O_2 concentrations, the Cu-ACE process enables lithography-free formation of porous, micro-elliptical, and concave inverted surface morphologies with increased effective surface area and multi-scale roughness. These features collectively contribute to SERS enhancement; concave inverted morphologies may additionally promote localized electromagnetic field confinement. Silver (Ag) films with thicknesses ranging from 30 to 90~nm were deposited by thermal evaporation, yielding strong and reproducible SERS responses under 660~nm excitation using crystal violet as a model analyte. A unified, experimentally measured limit of detection (LoD) of 10^{-11} M is reported. Enhancement factors on the order of 10^7-10^8 are achieved across the investigated Ag thickness range, indicating a broad thickness tolerance. Owing to its one-step, lithography-free chemical processing and compatibility with wafer-scale fabrication, the proposed Cu-ACE-based platform offers a practical route toward low-cost and large-area SERS substrates.

Keywords: Surface-enhanced Raman spectroscopy, Metal-assisted chemical etching, Inverted pyramidal structures

Graphical Abstract



Cu-assisted chemical etching transforms flat Si into inverted pyramidal microstructures, followed by Ag coating to form a scalable SERS substrate. The resulting concave morphology enables strong field enhancement (EF ~10^7–10^8) and sensitive detection of crystal violet down to 10^{-10} M.

Oral Abstracts

[Abstract:0447] [SERS/TERS/Plasmonics]

SERS-Based Label-Free Exosome Profiling for Acute Leukemia Detection Via Machine Learning

***Munevver Akdeniz*[1], *Zakarya Al Shaebi*[1], *Muzaffer Keklik*[2], *Omer Aydin*[3]**

[1]*Department of Biomedical Engineering, Erciyes University, Kayseri, 38039, Türkiye, NanoThera Lab, ERFARMA-Drug Application and Research Center, Erciyes University, Kayseri, 38280, Türkiye*
[2]*Department of Hematology, Faculty of Medicine, Erciyes University, 38039 Kayseri, Türkiye*
[3]*Department of Biomedical Engineering, Erciyes University, Kayseri, 38039, Türkiye, NanoThera Lab, ERFARMA-Drug Application and Research Center, Erciyes University, Kayseri, 38280, Türkiye, ERNAM-Nanotechnology Research and Application Center, Erciyes University, Kayseri, 38039, Türkiye, ERKAM-Clinical Engineering Research and Implementation Center, Erciyes University, Kayseri, 38030, Türkiye, Betül-Ziya Eren Genome and Stem Cell Center, Erciyes University, Kayseri, Türkiye*

Liquid biopsy has emerged as a minimally invasive and powerful approach for early detection and monitoring of cancer through analysis of tumor-derived biomarkers in bodily fluids such as blood, urine, and saliva. These fluids contain a wide range of components, including circulating tumor cells (CTCs), circulating tumor DNA (ctDNA), cell-free DNA (cfDNA), microRNAs, proteins, and exosomes. Among these, exosomes have gained particular attention due to their stability, abundance, and ability to reflect molecular characteristics of their parent cells. Exosomes are nanosized (30-150 nm) extracellular vesicles secreted by various cell types, carrying a complex cargo of nucleic acids, proteins, and lipids. They play a critical role in intercellular communication and are closely associated with cancer progression, metastasis, and immune regulation. Their presence in multiple physiological fluids and their protective lipid bilayer make them highly promising biomarkers for early diagnosis, disease monitoring, and evaluation of treatment response. Surface-enhanced Raman spectroscopy (SERS) is an advanced analytical technique that enhances Raman signals using plasmonic nanostructures, enabling highly sensitive and specific molecular characterization. In this study, exosomes were isolated from the serum of patients with acute myeloid leukemia (AML), Acute lymphoblastic leukemia (ALL) and healthy individuals, and SERS spectra were acquired using a gold nanoparticle (AuNPs) with positive charge-based substrate. Distinguishable spectral differences were observed between AML, ALL and healthy exosomes, particularly at Raman shifts around 726, 876, 1001, 1026, 1172, 1277 and 1530 cm^{-1}, corresponding to proteins, lipids, and nucleic acids. Distinct spectral fingerprints enabled group differentiation, and machine learning algorithms were used for classification. SVM and RF were applied to distinguish subtle differences among AML, ALL, and healthy exosomes, with RF achieving the highest accuracy of 99%. These results demonstrate that the proposed approach can reliably differentiate disease and healthy samples. Overall, integrating SERS with machine learning offers a rapid and promising strategy for acute leukemia exosome identification.

This work has been supported by Erciyes University Scientific Research Projects Coordination Unit under grant number # FDK-2025-14464.

Keywords: Exosomes, Acute leukemia, Surface-enhanced Raman Spectroscopy, Artificial intelligence

[Abstract:0456] [Materials]

Operando Raman Spectroelectrochemistry of Realistic Solid-State Batteries

***Raphael Ramos*, Elisa Grepin, Eliott Brun, Hélène Lotz, Olivier Raccurt, Sylvie Geniès**

Univ. Grenoble Alpes, CEA, Liten, 38000 Grenoble, France

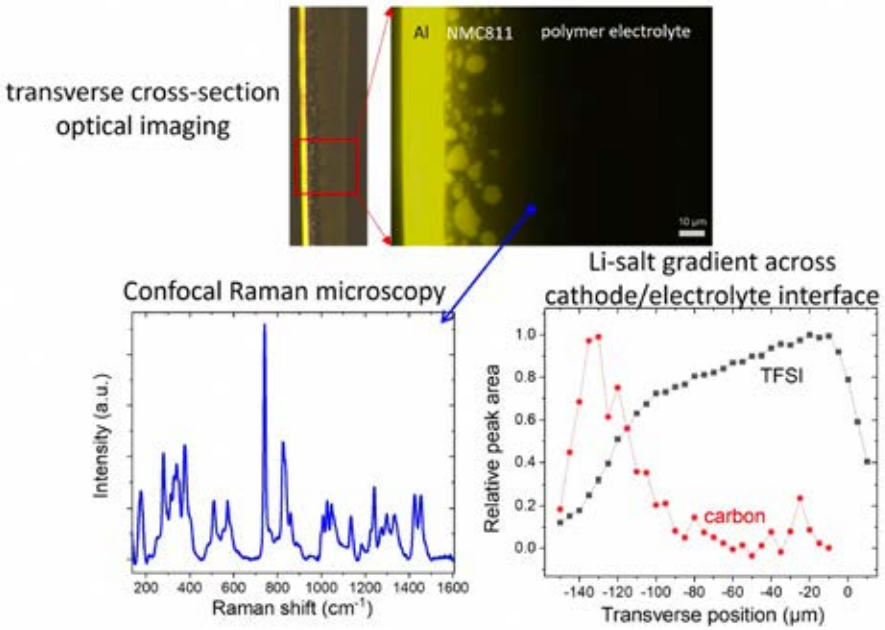
Raman scattering is powerful technique for battery materials research, probing the molecular structure of both electrodes, electrolytes, and their interfaces at relevant micrometer scale. It does however require direct optical access to those components, which prevents true operando interrogation of real batteries and dictates the use of model systems mimicking their behavior.

Our approach allows operando Raman characterization of solid-state battery cells and commercial electrodes arranged in a realistic configuration. We indeed leverage the sub-micrometer spatial resolution of confocal Raman microscopy to probe the transverse cross-section of battery cells. This configuration provides simultaneous and unobstructed optical access to the different battery components and their interphases (Fig. 1). We will present both the interest, limitations and challenges of this approach for different electrolyte types.

For the exemplary case of the interface between metallic lithium and polymer electrolyte, we will compare both the electrochemical and spectroscopic signatures obtained with a realistic cross-section configuration and with regular model system configurations.

Keywords: operando, battery, electrolyte

Figure 1



Confocal Raman microscopy of transverse cross-section of solid-state battery stack enables operando interrogation of electrodes, electrolyte and their interphases

[Abstract:0457] [SERS/TERS/Plasmonics]

From Lab to Field: Enhancing SERS Detection of Dipicolinic Acid Through Sampling-Relevant Chemical Activation Using Commercial Substrates and A Portable Raman Spectrometer

***Melike Sarıçam*, Serpil Harbeck, Melek Erol**

CBRN Defence Technologies Research Group, Materials and Process Technologies Vice Presidency, TÜBITAK MAM, Kocaeli, TÜRKIYE

Rapid and reliable detection of dipicolinic acid (DPA), a unique biomarker of Bacillus Anthracis, is of critical importance in chemical, biological, radiological, and nuclear (CBRN) threat assessment and bioterrorism response, where fast and field-deployable analytical tools are required. Major challenges in this context include not only sensitive detection, but also the effective recovery and transformation of trace bio-analytes from contaminated surfaces into detectable chemical signals. Inadequate recovery may lead to false-negative results, which directly compromises situational awareness and adversely affects CBRN preparedness and response strategies. This study addresses this challenge by focusing on maximizing DPA detectability through controlled chemical activation under sampling-relevant conditions. It is demonstrated that DPA detection via surface-enhanced Raman scattering (SERS) is governed by not only concentration but also protonation equilibria, counter-ion effects and coordination chemistry. Strongly acidic environments, particularly hydrochloric acid at low pH lead to a significant enhancement of SERS signals, likely due to chloride-mediated adsorption. In addition, calcium-containing conditions promote the formation of Ca–DPA complexes, yielding distinct and DPA-specific spectral features. To elucidate the critical role of sampling media composition in DPA detection, commercial Ag, Au, and hybrid Au/Ag-based SERS substrates were contaminated with increasing concentrations of DPA and systematically compared under identical experimental conditions using both benchtop and portable Raman spectrometers. Raman mappings, combined with multivariate analysis, reveal remarkable differences in signal enhancement, spectral uniformity, and reproducibility across substrates, emphasizing the influence of substrate architecture on analytical performance. Despite reduced sensitivity compared to benchtop measurements, reliable identification of DPA was achieved using a portable Raman spectrometer. Overall, this study integrates sampling-relevant chemical activation, commercial substrate benchmarking and the evaluation of SERS signals using a portable Raman spectrometer to establish a practical and scalable framework for DPA detection. The results provide a basis for further studies aimed at improving on-site detection approaches for surface-bound CBRN-related bioanalytes.

Keywords: SERS, bioterrorism, Bacillus Anthracis, DPA detection, portable Raman spectrometer, CBRN

[Abstract:0458] [Industrial/Societal Applications]

Discrimination of Ballpoint Pens and Analysis of Artificially Aged Document with Confocal Raman Spectroscopy

***Eda Kiriş*, Dilek Salkım Işlek, Erdoğan Köse**

Department of Science, Istanbul University-Cerrahpasa Institue of Forensic Sciences and Legal Medicine, Istanbul, Türkiye

One of the most common crimes encountered in forensic science is document forgery. Estimation of the time of a document's creation has a great importance. For this reason, studies using Raman spectroscopy increase in recent years due to its non-destructive nature, non-required of a sample preparation step, and its rapid analysis time. The aim of this study is to discrimination of ballpoint pens and analyze the dye in the structure of artificially aged ballpoint pen inks using Confocal Raman Spectroscopy to detect changes over time.

In the study, 12 ballpoint pens of different brands and models were randomly selected from the local market, and lines were drawn on standard A4 office paper using pens. A Vividia FM-120 digital magnifier was used to visually distinguish the pens. For artificial aging, the pens were artificially aged using a 300W UV lamp at a distance of 45 centimeters in 30-minute intervals for a total of 3 hours. A Renishaw Invia Confocal Raman Spectrometer was used for analysis. To minimize the fluorescence effect caused by the paper, a green laser with a wavelength of 532 nm was selected, and the parameters (exposure time, laser energy, accumulations) were optimized. Measurements were taken at 10 different points for each pen. After applying data preprocessing (subtract baseline and smooth) to the spectra, the spectral data were analyzed using Principal Component Analysis (PCA) and Hierarchical Cluster Analysis (HCA) by the OriginLab software.

The results of the analysis showed that crystal violet was present in the composition of the ballpoint pens. The pens for which Raman spectra were obtained were classified into three groups following PCA analysis. When HCA was applied to the pens, differentiation was achieved for all pens. Absolute intensity values were used to evaluate the results of the artificial aging analysis. As a result of artificial aging, it was determined that the 1620 cm^{-1} peak in the pens was more stable over time, while the 914 and 1584 cm^{-1} peaks exhibited time-dependent changes. PCA was applied to the obtained spectra, and differentiation was detected in samples with time differences.

Keywords: Raman Spectroscopy, Forensic Sciences, Ballpoint Pen, Discrimination, Artificial Ageing

[Abstract:0461] [SERS/TERS/Plasmonics]

Detection to Degradation: A SERS Strategy for Tackling Benzotriazole in Complex Water Matrices

***Arna Ghosh*[1], *Adrian Bohm*[1], *Valentin Ripka*[1], *Mario Lüdicke Ziegler*[1], *Juergen Popp*[2], *Dana Cialla-May*[2]**

[1]*Leibniz Institute of Photonic Technology, Member of Leibniz Health Technologies, Member of the Leibniz Centre for Photonics in Infection Research (LPI), AlbertEinsteinStraße 9, 07745 Jena, Germany*
[2]*Institute of Physical Chemistry and Abbe Centre of Photonics, Friedrich Schiller University Jena, Member of the Leibniz centre for Photonics in Infection Research (LPI), Helmholtzweg 4, 07743, Jena, Germany*

Benzotriazole (BTAH) and its methylated derivatives are commonly found in surface water because they are used as corrosion inhibitors in industrial cooling systems and de-icing of airplanes. [1] These compounds exhibit high water solubility, but reduced biodegradability. As a result, they can accumulate in aquatic environment and can cause chronic risk for ecosystem. In extreme cases, harmful concentrations up to 2.5 mg/L (~ 10-5 M) are found. Therefore, trace level detection is very important for all these compounds. To achieve such sensitive detection, SERS offers a powerful alternative to conventional analytical techniques. [2] Herein, we employ AgNPs (Fig.1a) as SERS substrate for direct detection of BATH and its methylated derivatives. The 787 cm-1 mode of BTAH is applied as marker mode to identify this molecule in wastewater after de-protonation performing SERS measurements in alkaline conditions (Fig.1b). Furthermore, a method to degrade BTAH catalytically using various silver-doped nanostructures (SiO2, ZnO and TiO2) and subsequent SERS detection is introduced. Significant decrease in intensity is observed by means of SiO2-based nanostructures. Thus, the SERS-based method shows huge potential being a rapid, cost-effective, and on-site analysis tool for trace level detection of micropollutants in water samples.

Acknowledgement: We thank the Federal Ministry of Research, Technology and Space, Germany (Bundesministerium für Forschung, Technologie und Raumfahrt, BMFTR) for supporting the project grant 03ZU1214EA.

References:

[1] Y. Jeong, Y. Lee, S. Nam, K. Kim, Environmental Research, 285, 122624 (2025).

[2] D. Cialla-May, A. Bonifacio, T. Bocklitz, A. Markin, N. Markina, S. Fornasaro, A. Dwivedi, T. Dib, E. Farnesi, C. Liu, A. Ghosh, J. Popp, Chem. Soc. Rev., 53, 8957-8979 (2024).

Keywords: SERS, water pollution, detection scheme

Silver nano- particles as SERS substrate, concentration dependent and degradation measurement of Benzotriazole in complex matrices

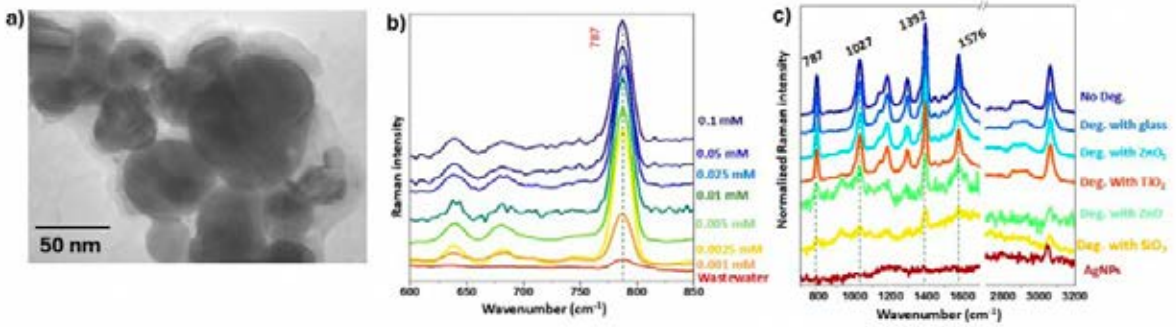


Figure 1. a) TEM image of AgNPs after BTAH exposure. b) Concentration dependent SERS spectra of BTAH extracted from wastewater. c) SERS spectra after degradation with various silver-doped nanostructures.

[Abstract:0465] [Biology/Biomedicine]

Light-Responsive Plasmonic Nanoparticle-Bacterial Biohybrids for Targeted and Multiplexed SERS Imaging

***Jorge Perez-Juste*, Isabel Pastoriza Santos**

CINBIO, Department of Physical Chemistry, Universidade de Vigo, Vigo, Spain

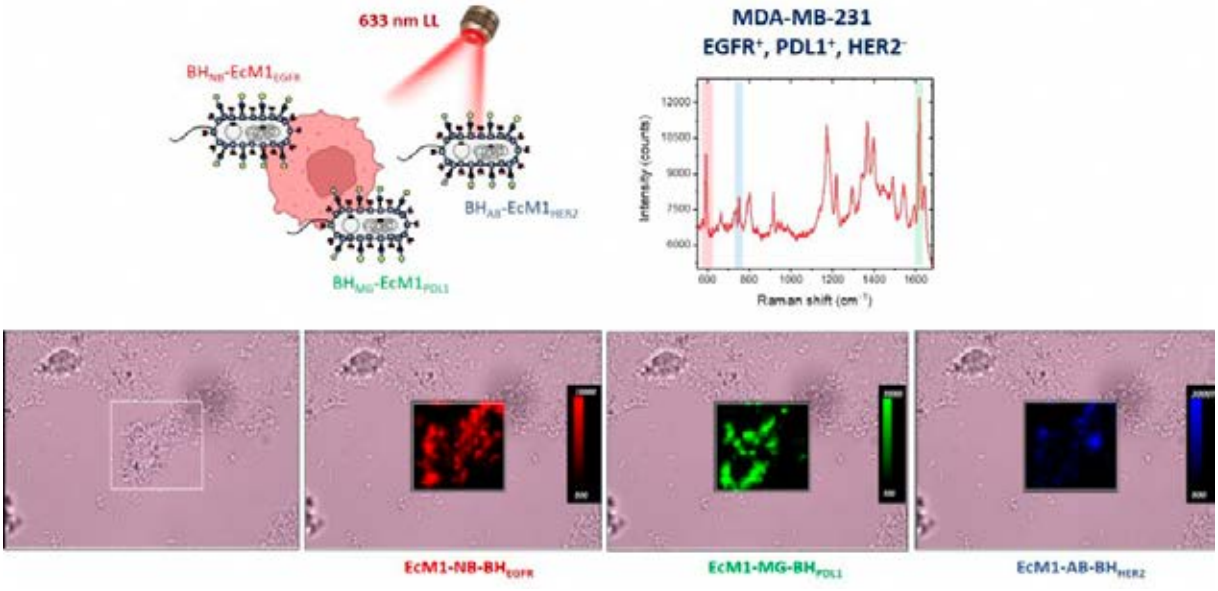
We report the development of bacterial biohybrids that combine non-pathogenic, genetically engineered *Escherichia coli* with plasmonic gold nanoparticles (AuNPs) to create a targeted and multiplexed SERS imaging platform (EcBHs). These living hybrid materials rely on: (i) programmable bacterial surface engineering for the selective display of binding moieties against tumour-associated biomarkers; (ii) covalent anchoring of Raman-encoded AuNPs to the bacterial surface through the SpyTag/SpyCatcher system, ensuring robust nanoparticle attachment while preserving bacterial viability and motility; and (iii) the plasmonic enhancement provided by AuNPs, enabling highly sensitive surface-enhanced Raman scattering (SERS) detection.

By engineering distinct bacterial populations expressing anti-EGFR, anti-HER2, and anti-PDL1 nanobodies, we demonstrate selective recognition of different cancer-associated membrane markers and achieve multiplexed imaging and immunophenotyping using a single excitation laser line (see Figure). In vitro studies confirmed efficient biohybrid assembly, preserved bacterial functionality, and specific binding to target cells. The resulting EcBHs act as actively targetable SERS probes that integrate bacterial motility, programmable molecular recognition, and spectrally encoded Raman readout within a single living platform.

This work establishes a versatile framework for bacteria-based plasmonic biohybrids for targeted molecular imaging, multiplexed cancer cell profiling, and SERS-guided interrogation of tumour heterogeneity.

Keywords: Bacterial biohybrids, Multiplexed imaging, Synthetic biology

Figure 1



Imaging biohybrid cell-adhesion by SERS

[Abstract:0466] [SERS/TERS/Plasmonics]

Label-Free Monitoring of Intracellular Pathways Via Surface-Enhanced Raman Scattering

***Deniz Yilmaz*[1], *Mustafa Culha*[2]**

[1]*Department of Genetics and Bioengineering, Faculty of Engineering and Natural Sceinces, Yeditepe University, Istanbul, Turkey*
[2]*Department of Chemistry and Biochemistry, College of Science and Mathematics, Augusta University, Augusta, Georgia, USA*

Elucidating intracellular pathways is fundamental to the development of effective biomedical interventions, including targeted drug delivery, biosensing, and molecular imaging. Although traditional analytical techniques, such as immunocytochemistry, Western blotting, and RNA sequencing, provide high specificity and selectivity, they are often limited by their destructive nature, complex sample preparation and extraction, and high operational costs. Consequently, there is a significant demand for non-invasive, high-sensitivity and selectivity methodologies that can monitor cellular dynamics in real-time.

Surface-enhanced Raman scattering (SERS) is a highly sensitive and non-destructive vibrational spectroscopy that can provide molecular fingerprint information from desired structures in the presence of noble metals. It requires minimal sample size and sample preparation methodology, and has water interference resistance. It has been widely employed across diverse scientific disciplines, ranging from food safety and agricultural monitoring to advanced applications in pharmacology and clinical medicine.

In this study, intracellular mechanisms were investigated by SERS using gold nanoparticles (AuNPs) as a SERS substrate. First, the cellular uptake of AuNPs was characterized by tracking SERS spectra in the presence of specific endocytosis inhibitors, allowing for the identification of different internalization pathways. For this purpose, various cell lines were exposed to inhibitors for clathrin-mediated endocytosis, caveolae-mediated endocytosis, and macropinocytosis prior to AuNP treatment. The intracellular SERS spectra were acquired from single living cells, and the resulting data were analyzed using principal component and linear discriminant analysis. The results demonstrated that significant spectral changes occur following the inhibition of different endocytic pathways. Subsequently, SERS was applied to characterize the biochemical changes associated with macrophage polarization. For this, RAW 264.7 cells were stimulated with lipopolysaccharide (LPS), and polarization was characterized by measuring nitric oxide and reactive oxygen species levels. This polarization process was then tracked via SERS at the single-cell level. The measurements revealed that macrophage activation can be monitored through significant changes in the intracellular SERS spectra. This study demonstrates that SERS enables the label-free, non-destructive monitoring of both AuNP endocytosis and LPS-induced macrophage activation, highlighting its potential as a robust tool for studying complex biological processes.

Keywords: SERS, Gold nanoparticles, endocytosis, macrophages

[Abstract:0467] [Biology/Biomedicine]

Beyond Histology: Detecting Endometrial Polyps Through Raman Spectroscopy

Andresa Dias[1], Maria Marques Félix[2], Dora Antunes[3], Clara Martins[4], Maria Paula Marques[4], Luis Alberto Esteves Batista de Carvalho[1], Maria João Carvalho[5], Ana Batista de Carvalho[1]

[1]Molecular Physical-Chemistry – LAQV/REQUIMTE, Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal
[2]Molecular Physical-Chemistry – LAQV/REQUIMTE, Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal, University of Coimbra, Faculty of Medicine, 3000-548, Coimbra, Portugal, Centre for Innovative Biomedicine and Biotechnology (CIBB), 3000-548 Coimbra, Portugal
[3]Molecular Physical-Chemistry – LAQV/REQUIMTE, Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal, Univ Coimbra, Coimbra Institute for Clinical and Biomedical Research (iCBR), area of Environment Genetics and Oncobiology (CIMAGO), and Institute of Biophysics, Faculty of Medicine, 3000-354 Coimbra, Portugal, Gynecology Department, Coimbra Local Health Unit, Portugal
[4]Molecular Physical-Chemistry – LAQV/REQUIMTE, Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal, University of Coimbra, Department of Life Sciences, 3000-456 Coimbra, Portugal
[5]Coimbra Institute for Clinical and Biomedical Research (iCBR) area of Environment Genetics and Oncobiology (CIMAGO), Faculty of Medicine, University of Coimbra, Coimbra, Portugal, Centre for Innovative Biomedicine and Biotechnology (CIBB), 3000-548 Coimbra, Portugal, Clinical Academic Center of Coimbra (CACC), 3000-354 Coimbra, Portugal, Gynecology Department, Coimbra Local Health Unit, Portugal,, Gynecology Clinic, Faculty of Medicine, University of Coimbra, Portugal, Faculty of Medicine, 3000 Coimbra, Portugal

Endometrial polyps are a common gynaecological disorder affecting women in pre- and post-menopause, carrying an increased risk of endometrial malignancy after menopause, especially in women presenting uterine bleedings. Nonetheless, given the low incidence of endometrial cancer in asymptomatic women, and the risks associated with the surgical procedure for their removal, most polyps can be kept under surveillance. However,currently, there is no consensus on the optimal management approach.

Endometrial cancer diagnosis is achieved by the histopathological analysis of the removed polyps or of a biopsy sample of the suspected lesion. Adding to the subjective nature of histopathology, endometrial biopsies are often jeopardised by low quality and low quantity samples, and by the absence of a standardised protocol, increasing the inter-observer variability.

In this context, Raman spectroscopy has emerged as a promising analytical technique that detects the vibrational signatures of the analyzed biological specimen. This study explores the analysis of hysteroscopic fluid, acting as a form of liquid biopsy, containing circulating cells and molecular biomarkers that reflect the biochemical microenvironment of the endometrium, spanning conditions from normal tissue, to polyp formation, hyperplasia and carcinoma.

The rationale for this approach is based on the detection of molecular alterations associated with polyp formation and respective risk factors. Raman spectroscopy enables the detection and quantification of these subtle biochemical changes without requiring external labels or destructive sample preparation.

The first approach to this study involved a comparative spectroscopic analysis of hysteroscopic fluid samples from women with and without (control) endometrial polyps. Distinct spectral fingerprints were observed between the two groups. PCA was subsequently applied, revealing major differences in DNA, lipid, and protein-related signals in PC1 and PC2.

These preliminary results support the future application of liquid biopsies coupled with Raman spectroscopy for the detection of endometrial polyps and monitoring of therapeutic response in endometrial pathologies. It is expected prospectively in this study that this technique will be able to evaluate polyp-related malignancy and response to therapy using hysteroscopic fluids.

Keywords: Endometrial Polyps, Raman Spectroscopy, Hysteroscopic Fluid, Diagnosis

[Abstract:0469] [SERS/TERS/Plasmonics]

SERS-Based Analysis of Biological Fluids for Liquid Biopsy Applications

Valentin Toma[1], Anca Onaciu[1], Rareș-Mario Borșa[3], Luca David[1], Dragoș-Ioan Olariu[4], Septila Renata[4], Gabriela Fabiola Stiufiuc[5], Brindusa Dragoi[6], Rares Stiufiuc[2]

[1]Department of NanoSciences, Institute of BioMedical Research – MedFUTURE, Louis Pasteur 4-6, 400349, Cluj-Napoca, Romania
[2]Department of Pharmaceutical Physics & Biophysics, Faculty of Pharmacy, "Iuliu Hatieganu" University of Medicine and Pharmacy, Pasteur 6, 400349 Cluj-Napoca, Romania
[3]Department of Maxillofacial Surgery and Implantology, "Iuliu Haţieganu" University of Medicine and Pharmacy, Cardinal Iuliu Hossu 37, 400029 Cluj-Napoca, Romania
[4]Nanotechnology Laboratory, TRANSCEND Department, Regional Institute of Oncology, 2-4 General Henri Mathias Berthelot, 700483 Iasi, Romania
[5]Faculty of Physics, "Babes-Bolyai" University Cluj-Napoca, 1 M. Kogalniceanu, 400084, Romania
[6]Faculty of Chemistry, "Alexandru Ioan Cuza" University of Iasi, 11 Carol I Blvd., 700506 Iasi, Romania

Surface-enhanced Raman scattering (SERS) has emerged as a powerful analytical technique in the evolving landscape of liquid biopsy, enabling rapid, label-free, and ultrasensitive molecular characterization of complex biological samples. By exploiting localized surface plasmon resonance in metallic nanostructures, SERS significantly amplifies inherently weak Raman signals, allowing detection of low-abundance biomolecules.

Our group has developed SERS-based approaches for the investigation of various pathological conditions (e.g. ulcerative colitis, prostate, breast, oral and renal cancers) using biological fluids collected through minimally invasive procedures, including blood serum and plasma, urine and saliva. The use of solid substrates based on plasmonic silver nanoparticles developed within our group enhances signal stability, sensitivity, and inter-sample reproducibility, addressing key challenges for translational applications. The resulting spectral fingerprints are dominated by contributions from metabolites such as purines, proteins, lipids, and carotenoids, which reflect disease-associated biochemical alterations. These molecular signatures enable discrimination between healthy and diseased states, with improved classification performance achieved through multivariate statistical analysis and machine learning algorithms.

Recent efforts have extended the applicability of SERS to the analysis of DNA methylation patterns, cellular lysates and extracellular vesicles, particularly exosomes, which carry DNA, RNA, and protein cargo relevant to tumor progression and intercellular communication.

Overall, SERS-based liquid biopsy represents a versatile and promising platform for non-invasive diagnosis, patient stratification, and disease monitoring, supporting advances in precision and personalized medicine.

Acknowledgments:

This work was supported by a H2020 project - Coordination and support action, WIDESPREAD-06-2020 (ERA-Chairs), no. 952390/09.06.2020 (www.esei-biomed.eu).

Keywords: liquid biopsy, SERS, biofluids

[Abstract:0470] [Theory/Computation]

Accelerating Raman Spectroscopy Imaging Via Fine-Tuned Diffusion Models for Sparse Data Reconstruction

***Roozbeh Bonakdar*[1], *Muhammet Baki Karakus*[2], *Arda Inanç*[2], *Bora Akgun*[2], *Bora Akgun*[3], *Mehmet Burcin Unlu*[4]**

[1]*Department of Electrical and Electronics Engineering, Özyeğin University, Istanbul, Turkey*
[2]*Department of Physics, Boğaziçi University, Istanbul, Turkey*
[3]*Center for Life Sciences and Technologies, Boğaziçi University, Istanbul, Turkey*
[4]*School of Engineering, Özyeğin University, Istanbul, Turkey*

Raman spectroscopy imaging is a powerful non-destructive analytical technique, but its widespread application is often hindered by inherently long acquisition times. To overcome this limitation, sparse sampling followed by computational reconstruction offers a promising solution. In this work, we present Diff-Raman, a novel approach leveraging generative diffusion models to reconstruct highly undersampled Raman images. By fine-tuning a pre-trained OpenAI Guided-Diffusion model on a custom, robust dataset of over 2,690 Raman topological maps, we bridge the significant domain gap between natural image priors and scientific spectroscopic data.

Our methodology evaluates reconstruction performance across varied structural characteristics by selecting two distinct spectral peaks from the dataset: one representing maximum variance and another chosen randomly. These peaks are used to generate corresponding PCA score maps and peak-intensity images, establishing a comprehensive baseline for structural and spectral evaluation. To rigorously test our model, we simulate undersampling by explicitly deleting vertical columns from the spatial maps. This is achieved using two distinct strategies: uniform column deletion along the y-axis and completely random column deletion, mimicking realistic rapid-scanning scenarios.

We benchmark Diff-Raman against conventional interpolation-based methods typically used for sparse data recovery. Our results clearly demonstrate that the fine-tuned diffusion model drastically outperforms traditional techniques. Specifically, Diff-Raman establishes clear superiority across key quantitative and qualitative metrics, showing unprecedented improvements in structural similarity (SSIM), peak-intensity fidelity, and overall visual quality.

Ultimately, Diff-Raman aims to redefine the limits of Raman imaging speed. By reliably reconstructing complex topological and chemical information from highly sparse data, this framework will enable real-time tracking of dynamic chemical processes and facilitate high-throughput screening without compromising spatial resolution or spectral integrity.

Keywords: Raman spectroscopy, Image reconstruction, Sparse data recovery, Computational spectroscopy

[Abstract:0472] [Novel Approaches]

Interfacial Vibrational Spectroscopic Insights into Membrane Disruption Using Antimicrobial Peptides

***Montserrat Roman Quintero*[1], *Vincent Hempel*[2], *Mark Mero*[3], *Zsuzsanna Heiner*[1]**

[1]*School of Analytical Sciences Adlershof (SALSA), Department of Chemistry, Humboldt-Universität zu Berlin, 12489 Berlin, Germany*
[2]*Faculty of Mathematics and Natural Sciences, Department of Chemistry, Humboldt-Universität zu Berlin, 12489 Berlin, Germany*
[3]*Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany*

The rise of antibiotic-resistant pathogens poses a significant global health challenge, underscoring the need for alternative antimicrobial strategies beyond traditional antibiotics. One promising strategy is the use of functional surface coatings that inhibit bacterial adhesion and growth, especially in high-contact areas like healthcare facilities and public infrastructure. This study examines interfacial peptide–membrane interactions using the antimicrobial peptide Aurein 1.2 as a model system to elucidate mechanisms relevant to antimicrobial surface design.

We use a multimodal vibrational spectroscopy method to investigate molecular structure and dynamics across various length scales. Vibrational Sum Frequency Generation (VSFG) spectroscopy, a label-free, interface-specific nonlinear optical technique, detects molecular ordering and symmetry disruptions at lipid interfaces with monolayer sensitivity. Additionally, nano-FTIR spectroscopy offers nanoscale resolution, enabling spatially resolved vibrational analysis of membrane heterogeneity.

Here, we systematically investigate peptide-induced membrane degradation using VSFG to monitor real-time monolayer interactions with the peptide, and nano-FTIR for solid-supported bilayers. Varying peptide concentrations allow us to observe membrane disruption by detecting changes in the vibrational modes of lipid alkyl chains and headgroups. VSFG spectra show notable shifts in interfacial vibrational signatures, suggesting decreased lipid order and compromised membrane e integrity. These results, i.e., changes in vibrational frequency, intensity, and linewidth, indicate alterations in molecular conformation and environment. Real-time study of the interaction enabled detection of the initial steps of membrane folding into the model membranes. Furthermore, nano-FTIR measurements further support these findings by providing nanoscale evidence of lipid headgroup disturbance and local structural disorder.

Together, this work demonstrates how advanced vibrational spectroscopies can deliver molecular-level insight into antimicrobial peptide activity at interfaces. The combined approach establishes a powerful spectroscopic framework for elucidating mechanisms of membrane disruption and guiding the development of next-generation antimicrobial coatings.

Keywords: VSFG spectroscopy, nano-FTIR spectroscopy, membrane, antimicrobial peptides

Oral Abstracts

[Abstract:0479] [Novel Approaches]

Coherent Raman Spectroscopy for Buried Interfaces Via Spatiotemporal Field Engineering

***Chengxiang Jin*[1], *Tsuneto Kanai*[2], *Atsunori Sakurai*[2], *Toshiki Sugimoto*[2]**

[1]*Graduate Institute for Advanced Studies, SOKENDAI, Okazaki, Aichi 444-8585, Japan*
[2]*Department of Materials Molecular Science, Institute for Molecular Science, Okazaki, Aichi 444-8585, Japan*

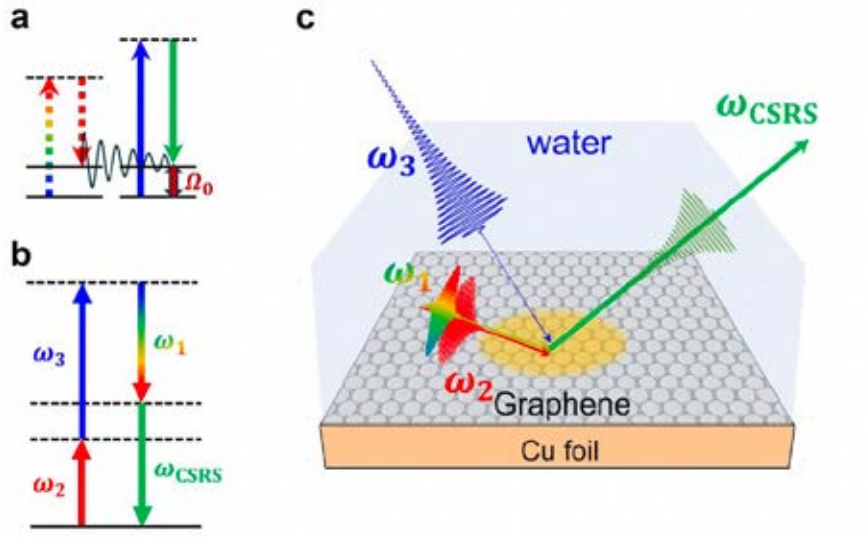
Buried solid–liquid interfaces play a central role in a wide range of chemical processes, yet their direct spectroscopic observation without surface enhancement, such as that provided by metallic nanoparticles or plasmonic nanostructures, remains challenging. Coherent Raman scattering (CRS) offers strong signal enhancement through stimulated third-order nonlinear interactions and allows the use of visible and near-infrared excitation that propagates through bulk liquids with minimal absorption. However, CRS is inevitably accompanied by a large vibrationally non-resonant background (NRB) originating from the bulk liquid, which coherently builds up over the coherence length and overwhelms interfacial contributions. Here, we report an interface-sensitive CRS approach based on simultaneous spatial and temporal focusing (SSTF). The principle of the method and the experimental geometry are illustrated in Fig. 1a–c. In SSTF, a spatially dispersed ultrashort pulse recombines only near the focal plane, resulting in localized temporal compression. While SSTF has been widely applied in incoherent nonlinear microscopy, its role in coherent optical processes has remained largely unexplored.

Using single-layer graphene on Cu immersed in D_2O as a model buried interface (Fig. 1c), we demonstrate pronounced suppression of bulk-liquid NRB together with enhanced interface sensitivity. In a conventional focusing geometry, the NRB from bulk liquid dominates the signal and obscures the graphene vibrational response. In contrast, under SSTF conditions, the characteristic dispersive feature of the graphene G band remains clearly visible at the buried interface. Quantitative analysis shows that the bulk-liquid NRB is reduced to approximately 7% of that in the conventional case.

These results establish SSTF as an effective approach for suppressing bulk NRB and enhancing interface sensitivity in CRS, opening a route to in situ vibrational spectroscopy of buried interfaces under realistic conditions, including operando electrochemical environments.

Keywords: coherent Raman spectroscopy, spatiotemporal focsing, buried solid–liquid interfaces, electrochemical interfaces, operando spectroscopy

Fig. 1. The principle of the method and the experimental geometry



(a) Optical process of vibrationally resonant coherent Stokes Raman scattering. (b) Optical process of non-vibrationally resonant background (NRB) signal. (c) Schematic illustration of CRS measurements under electrochemical conditions.

[Abstract:0481] [Theory/Computation]

Continual Learning Strategies for Sequential Pathogen Update in Raman Spectroscopy-Based Identification

Marwan A. Farag[1], Helal A. Suleiman[2], Rami Zewail[3], Amr Nassrallah[4], Ahmed Abdel-Mawgood[4], Sameh Awad[5], Badawi Anis[6], Samir El-Mashtoly[7]

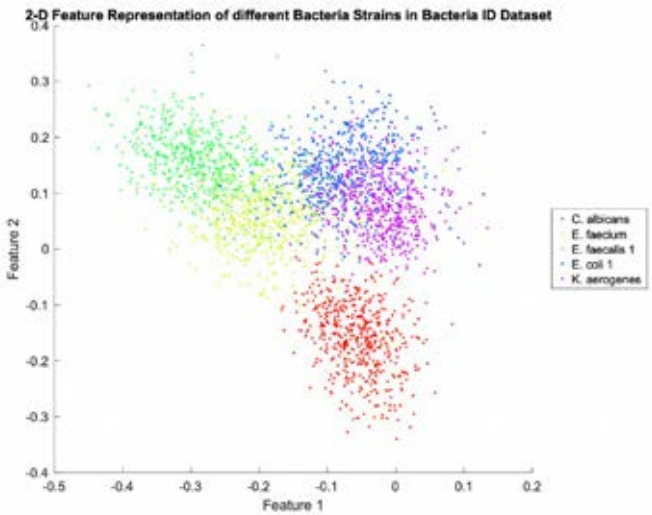
[1]Faculty of Computer Science & Information Technology, Helwan National University, Cairo, Egypt
[2]Faculty of Computers and Artificial Intelligence, Capital University, Egypt
[3]Department of Computer Science & Engineering, Egypt-Japan University of Science and Technology (E-JUST), New Borg El Arab, Alexandria, Egypt
[4]Biotechnology department, Faculty of Basic and Applied Science, E-JUST, New Borg El-Arab, Egypt
[5]Department of Dairy Science and Technology, Faculty of Agriculture, Alexandria University, Egypt
[6]Spectroscopy Department, Physics Research Institute, National Research Centre (NRC), Giza, Egypt
[7]Leibniz Institute of Photonic Technology, Albert-Einstein-Straße 9, Jena, Germany

Existing AI-driven Raman spectroscopy often relies on static supervised learning that struggles with "catastrophic forgetting" during sequential task updates. To address this, we evaluate various continual learning algorithms integrated with a ResNet backbone to enable the addition of new bacterial pathogens without total retraining. We compared Elastic Weight Consolidation (EWC), Synaptic Intelligence (SI), and Learning without Forgetting (LwF) for their ability to protect pathogen-specific weights.

RESULTS: As shown in Table 1, EWC achieved the highest stability with a final accuracy of 99.34%, outperforming LwF (98.67%) and SI (98.34%). The 2-D feature representations (Figure 1) demonstrate high intra-class cohesion and inter-class separation for pathogens such as E. coli and K. aerogenes, validating the backbone's feature discriminability. Furthermore, the sharp diagonal dominance in the identification matrices (Figure 2) confirms the framework's ability to shield pathogen-specific weights via the Fisher Information Matrix, successfully retaining knowledge across sequential tasks without total retraining.

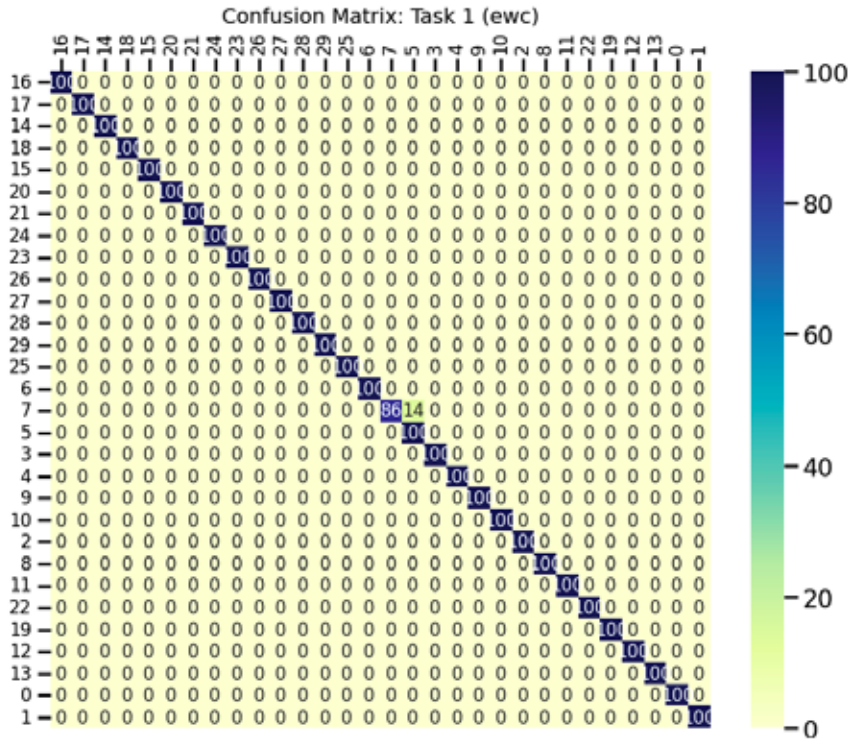
Keywords: Raman Spectroscopy, Continual Learning, ResNet, Feature Representation

Figure1



2-D feature representation of diverse bacterial pathogens

Figure2



Confusion matrix for pathogen identification using EWC across sequential tasks, showing sharp diagonal dominance indicative of successful parameter protection.

Table1

Algorithm	Final Accuracy (%)	Task Retention Outcome
Elastic Weight Consolidation (EWC)	99.34%	Superior task stability
Learning without Forgetting (LwF)	98.67%	High general feature preservation
Synaptic Intelligence (SI)	98.34%	Minor decision boundary drift

Performance Comparison of Continual Learning Algorithms.

[Abstract:0485] [Biology/Biomedicine]

Multimodal Raman and AFM-IR Nanospectroscopy of Plasma Membrane Vesicles Reveals Cell-Origin Dependent Membrane Composition

***Katarzyna Pogoda*, Jagoda Orleanska Pietras**

Institute of Nuclear Physics PAN

The plasma membrane is a dynamic biological interface responsible for molecular transport, signal transduction, and communication between the cell and its environment. Understanding its molecular composition in a native state remains challenging because the complex intracellular environment often interferes with spectroscopic analysis. Giant plasma membrane vesicles (GPMVs), which are cell-derived membrane blebs preserving the native lipid and protein composition of the plasma membrane, provide a valuable model system for investigating membrane organization.

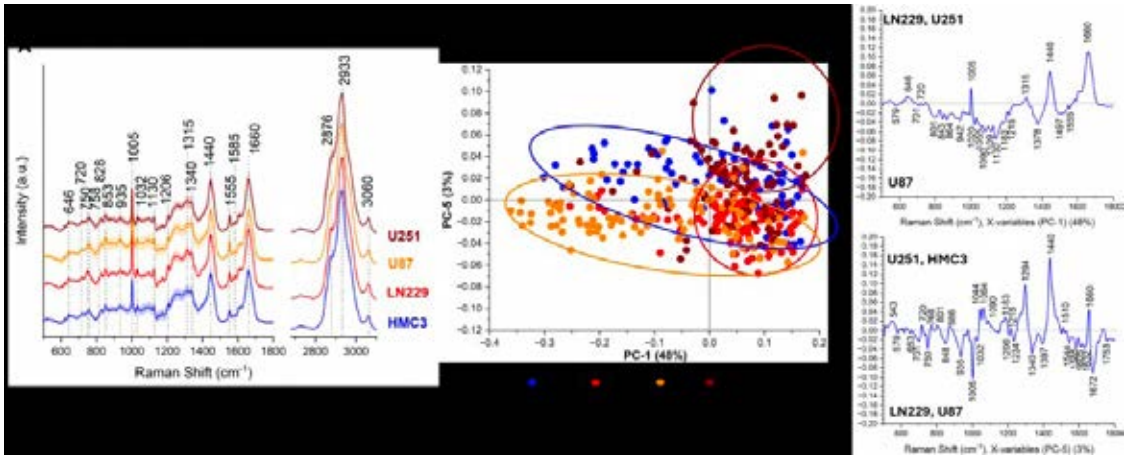
In this work, Raman spectroscopy was applied for label-free molecular characterization of GPMVs isolated from microglial (HMC3) and glioblastoma (LN229, U87, U251) cell lines. Raman spectra were recorded in the 400–3100 cm^{-1} range and revealed characteristic vibrational bands associated with phospholipids, proteins, and membrane-associated biomolecules (Fig. 1A). Spectral analysis demonstrated significant differences in biochemical composition between vesicles derived from different cellular origins. In particular, variations were observed in the intensity of phospholipid bands (~720 cm^{-1}), protein-related phenylalanine vibrations (~1005 cm^{-1}), and lipid unsaturation markers (~1660/1440 cm^{-1}).

Chemometric analysis of Raman spectra enabled clear discrimination of vesicles according to their cellular origin, highlighting differences between vesicles derived from normal microglial and cancerous glioblastoma cells (Fig. 1B). Complementary nanoscale information about membrane composition was obtained using AFM-IR spectroscopy, confirming variations in lipid, protein, and carbohydrate contributions at the nanoscale level.

The presented multimodal spectroscopic approach offers new opportunities for studying native membrane organization and disease-related alterations in plasma membrane composition.

Keywords: Raman spectroscopy, AFM-IR, plasma membrane, giant plasma membrane vesicles, chemometrics

Figure 1. Raman spectroscopic characterization of giant plasma membrane vesicles (GPMVs) derived from microglial and glioblastoma cells.



[Abstract:0489] [SERS/TERS/Plasmonics]

Detection of Chemical Warfare Agent Simulants on Commercial Substrates Via Surface-Enhanced Raman Spectroscopy

***Serpil Harbeck*[1], *Melek Erol*[1], *Melike Sarıçam*[1], *Ferda Gönülkırmaz*[1], *Tülay Durmuş*[2]**

[1]*CBRN Defence Technologies Research Group, Materials and Process Technologies Vice Presidency, TÜBITAK MAM, Kocaeli, TÜRKIYE*
[2]*Chemistry Department, Düzce University, 81010 Düzce, TÜRKIYE*

The sensitive and selective detection of chemical warfare agents (CWAs) on contaminated surfaces is critically important for CBRN defence and environmental safety. Various techniques, including fluorescence, colorimetric methods, electrochemical sensing, chemical sensors and surface-enhanced Raman spectroscopy (SERS), have beenproposed for CWA detection. Among these, SERS enables highly sensitive, real-time, and on-site detection at trace levels. In this study, the detection capabilities of various commercial SERS substrates for different classes of CWAs were investigated using representative simulants. Specifically, SERS-based detection of two selected CWA simulants, dimethyl 4-nitrophenylphosphate (DMNP) as a nerve agent simulant and 2-chloroethyl ethyl sulfide (2-CEES) as vesicant simulant- was performed using commercially available substrates. Metrohm Ag and Au P-SERS, Silmeco Au and Ag, and SERSitive Ag and Au–Ag substrates were systematically contaminated with definedamounts of the analytes. SERS measurements were conducted using excitation wavelengths of 532 nm and 785 nm to evaluate the influence of excitation conditions on signal enhancement. The results reveal that both substrate composition and excitation wavelength critically affect SERS performance. In particular, DMNP was more reliably detected under 785 nm excitation across all substrates, whereas its detection at 532 nm was limited, especially on Metrohm Au and Silmeco Au–Ag substrates. In contrast, the SERS response of 2-CEES exhibited a different trend. These findings indicate that signal intensity is strongly dependent on chemical structure, excitation wavelength, and substrate type. The observed differences can be attributed to inherent variations in the chemical structures of the analytes, which influence their adsorption behaviour, surface affinity, and Raman scattering efficiency. DMNP, as an organophosphorus compound, and 2-CEES, as a sulfur-containing mustard simulant, interact differently with plasmonic surfaces, leading to analyte-specific SERS responses as a function of experimental parameters. As a result, none of the commercial substrates examined in this study were capable of simultaneously detecting analytes representing both CWA classes.

Keywords: Chemical warfare agents, detection, SERS, commercial SERS substrates, Raman

Oral Abstracts

[Abstract:0492] [Planetary/Geosciences]

Diverse Mineralogies Characterized with SuperCam Raman and Luminescence in Jezero Crater

Elise Clave[1], Jose Antonio Manrique[2], Olivier Beyssac[3], Ann Martha Ollila[4], Erwin Dehouck[1], Sofia Julve[2], Ivan Reyes[2], Kristin Rammelkamp[5], Leire Coloma[6], Olivier Forni[7], Guillermo Lopez Reyes[2], Paolo Pillieri[7]

[1]LGL, U. Claude Bernard, Lyon, France
[2]ERICA, University of Valladolid, Valladolid, Spain
[3]IMPMC, Paris, France
[4]LANL, NM, USA
[5]DLR-WR, Nerlin, Germany
[6]UPV/EHU, Bilbao, Spain
[7]IRAP, Toulouse, France
[8]University of Hawaii, USA
[9]Purdue University, Indiana, USA

The SuperCam instrument [1,2,3] has been operating on Mars for over five years, demonstrating the significant capabilities of Raman spectroscopy, as well as time-resolved luminescence spectroscopy (TRLS) for in situ mineralogical characterization. To date, seven mineral classes have been identified unequivocally with SuperCam Raman: sulfates, Na-perchlorate, carbonates, olivines, apatite, pyroxenes, feldspars and quartz, plus the detection of an OH-band attributed to serpentine [4, 5, 6, 7]. Moreover, variable geochemistry was observed within these mineral groups: Fe-Mg carbonates of variable compositions [8,9] as well as Ca-carbonate; Ca-sulfate of different hydration levels (anhydrite type II and bassanite) [10]. Composition of olivine solid solution was also studied using Raman data [11, 12, 13]. Despite not being a mineralogical technique, a luminescence signature was observed, that we could only explain by the presence of Cr3+ in corundum, leading to the first in situ detection of this phase on Mars.13.

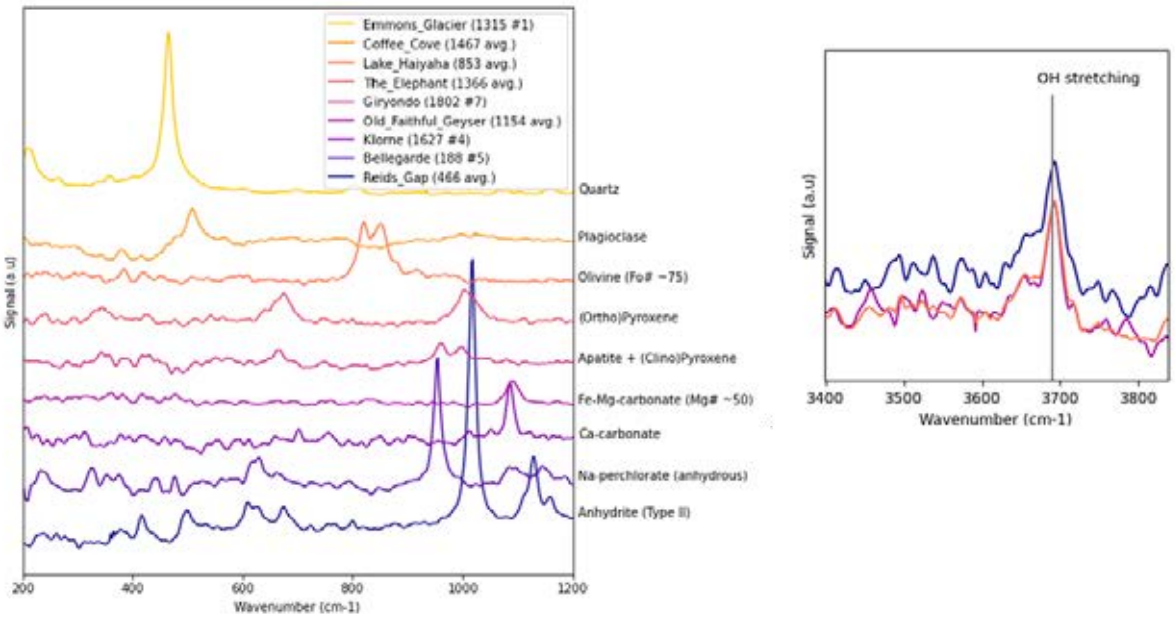
In a nutshell, SuperCam Raman assisted in the unequivocal identification of different minerals on Mars, linking these detections to astrobiologically relevant processes in Jezero Crater, like the possible hydrothermal origin of the quartz [7], or the alteration phases detected in Neretva Vallis, where the mission acquired the best potential biosignatures to date [14].

References:

1, Maurice et al., SR, 2021; 2. Wiens et al., SR, 2021; 3. Manrique et al., SR, 2021; 4. Lopez-Reyes et al., JGRP 2025; 5. Quantin-Nataf et al., Science, revised; 6. Comellas et al., submitted; 7. Beck et al., EPSL, 2025; 8. Clavé et al., JGRP 2023; 9. Clavé et al., JGRP revised; 10. Mandon et al., in prep.; 11. Beyssac et al., JGRP, 2023; 12. Beyssac et al., EPSL, 2026; 13. Lopez-Reyes et al., in prep.; 14. Ollila et al., GRP, in prep; 15. Hurowitz et al. Nature 2025

Keywords: Mars 2020, SuperCam, Jezero, Perseverance

Relevant detections



Example of Raman spectra collected by SuperCam

Oral Abstracts

[Abstract:0495] [Theory/Computation]

Nanographenes' Shapes: Effects of Molecular Geometry on Raman Spectra From Density Functional Theory

***Gianluca Serra*[1], *Andrea Lucotti*[1], *Akimitsu Narita*[2], *Ji Ma*[3], *Xinliang Feng*[4], *Matteo Tommasini*[1]**

[1]*Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta", Politecnico di Milano, Milan, Italy*
[2]*Organic Carbon and Nanomaterials Unit, Okinawa Institute of Science and Technology Graduate University, Okinawa, Japan*
[3]*College of Materials Science and Optoelectronic Technology and Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing, China*
[4]*Center for Advancing Electronics Dresden (cfaed) & Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Dresden, Germany, Max Planck Institute of Microstructure Physics, Halle, Germany*

Nanographenes, namely large polycyclic aromatic hydrocarbons, have attracted significant attention due to their unique optical and electronic properties. Since these properties depend on molecular dimension, shape, and edge-topology, organic chemistry has built a growing zoo of differently shaped nanographenes. The zoo recently included peculiar geometries, such as porous, wavy, and non-Kekuléan nanographenes, as well as nanographenes with high aspect ratio, also known as graphene nanoribbons.

Raman spectroscopy is an invaluable tool for the characterization of novel nanographenes: when complemented by quantum chemical calculations, it helps support their successful synthesis. We measured and calculated the Raman spectra of several nanographenes, with a particular focus on peculiar shapes, collecting a consistent experimental and computational dataset. This, in turn, allowed us to ask whether the effect of different geometrical features on nanographenes' Raman spectra could be framed into simple geometry-spectrum relationships. In doing so, we are motivated by a desire to increase the capabilities of Raman spectroscopy as a characterization tool for nanographenes.

We thus perform a systematic re-examination of measured and computed Raman spectra of more than fifteen nanographenes obtained over the last five years, including porous, wavy, and non-Kekuléan geometries as well as graphene nanoribbons. Aided by density functional theory calculations, we discuss the effect of geometrical features on the position and intensities of the most intense Raman bands. We find that different geometrical features affect the widely known D and G bands in different ways, with the D band being the most sensitive to molecular geometry within our data set. Taking advantage of such a discussion, we define a set of practices to calculate the Raman spectra of novel nanographenes within density functional theory.

Keywords: nanographenes, molecular geometry, density functional theory

[Abstract:0497] [Coherent Raman Imaging]

Visualization of Topical Drug Delivery with Label-Free Chemical İmaging

***Natalie Belsey*[1], *Dimitrios Tsikritsis*[1], *Panagiota Zarmpi*[2], *Jean Luc Vorng*[1], *Vasundhara Tyagi*[1], *Alex Dexter*[1], *Anukrati Goel*[2], *Richard Guy*[3]**

[1]*Chemical & Biological Sciences Department, National Physical Laboratory, Hampton Road, Teddington, TW11 0LW. UK*
[2]*School of Chemistry & Chemical Engineering, University of Surrey, Guildford, GU2 7XH, UK.*
[3]*Department of Life Sciences, University of Bath, Bath, BA2 7AY, UK.*

Stimulated Raman scattering (SRS) microscopy is capable of real-time examination of formulated products and their permeation into the skin, allowing the detailed, time resolved investigation of chemical absorption. The high sensitivity modulation transfer detection mechanism permits imaging free from emitted fluorescence, with the added benefit that the signal intensity is linear with concentration, simplifying quantitative analysis. SRS has shown excellent promise as a tool for the study of topical drug formulations themselves, in addition to the "metamorphosis" of applied formulations on skin and the real-time disposition of actives and excipients, including penetration pathway and nanoparticle distribution. In addition to unique mechanistic information, it provides a means of assessing topical drug bioavailability and bioequivalence. SRS can be performed simultaneously to other optical imaging modalities such as second harmonic generation (SHG) and fluorescence microscopies to image connective tissues and other endogenous species. Workflows have also been developed to perform correlative SRS-SHG-secondary ion mass spectrometry imaging (SIMS). This combination of spectroscopic imaging approaches facilitates powerful visualisation, combining high chemical specificity and sensitivity with sub-micron spatial resolution.

Keywords: Stimulated Raman scattering (SRS) microscopy, topical drug delivery, pharmaceuticals, tissue imaging

Fig 1

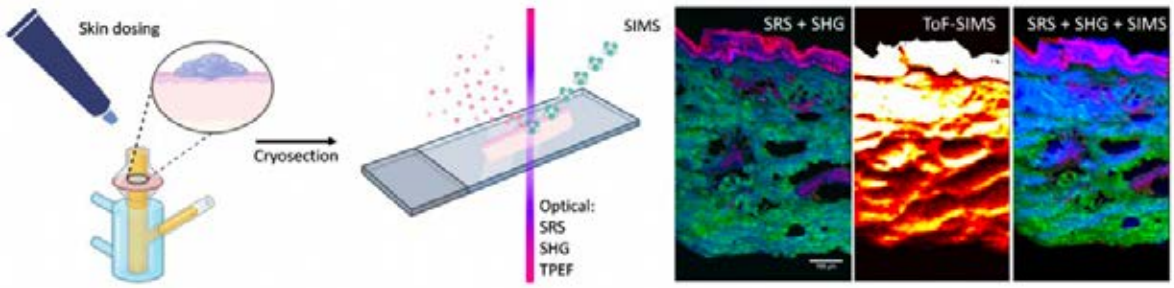


Figure 1: Methodology and example data from combining non-linear optical microscopies with mass spectrometry imaging for high resolution visualisation of drug distribution within the skin. N. A. Belsey et al. Journal of Controlled Release (2023) 364, 79-89.

Oral Abstracts

[Abstract:0498] [Coherent Raman Imaging]

Burst-Mode Femtosecond Lasers for Enhanced Stimulated Raman Spectroscopy

Yaren Sarıboğa

Özyeğin Üniversitesi

We present a theoretical and computational framework for applying burst-mode femtosecond laser excitation to stimulated Raman spectroscopy (SRS), targeting signal enhancements beyond what conventional single-pulse schemes permit.

Two complementary models are developed and compared numerically. A semiclassical coupled-wave model describes stimulated Raman gain under the undepleted-pump approximation, yielding standard exponential Stokes amplification $I_S(L) = I_S(0)\exp(g_R I_p L)$, but is limited to intensity-only dynamics with no phase information. For burst-mode excitation, a coupled nonlinear Schrödinger equation (NLSE) framework is required, incorporating group-velocity dispersion, self- and cross-phase modulation, and a convolution-based Raman response function that retains inter-pulse vibrational memory.The central result is coherent vibrational accumulation: when the intra-burst pulse spacing Δt is shorter than the molecular dephasing time T2, successive pulses drive the vibrational coordinate constructively. The amplitude after n pulses follows a geometric series with ratio $r = \exp(-\Delta t/T2)$, converging to a steady-state enhancement $|Q_\infty|^2 = |Q0|^2 / (1 - \exp(-\Delta t/T2))^2$. Simulations use a C–H stretch mode ($\Omega vib = 2900\ cm^{-1}$, $T2 \approx 1.06$ ps) with ten 50 fs pulses separated by 1 ps, tuned to match T2. Pulse-by-pulse results confirm cumulative Stokes enhancement across the burst, with vibrational coherence $|Q|$ building in discrete steps between pulses. The coupled-wave scheme achieves +0.19% Stokes gain, while the NLSE simulation captures full field-dependent dynamics including spectral broadening from SPM and XPM (pump: 3.09 → 5.06 THz; Stokes: 3.09 → 5.56 THz).A further capability demonstrated is hyper-spectral phase control: introducing a linearly incrementing inter-pulse phase offset $\Delta\varphi$ shifts the effective pump frequency comb, enabling motion-free spectral scanning across the Raman resonance without tuning the laser wavelength. This provides a path to high-resolution vibrational imaging at fixed laser frequency.

These results establish burst-mode femtosecond FSRS as a route to approximately two orders of magnitude signal enhancement over conventional single-shot FSRS, with additional capabilities including single-burst time-resolved Raman movies of irreversible processes and mode-selective vibrational filtering via intra-burst timing control.

Keywords: Stimulated Raman Spectroscopy, Burst-Mode Lasers, Femtosecond Pulses, Coherent Accumulation, Nonlinear Optics

Oral Abstracts

[Abstract:0499] [Coherent Raman Imaging]

Chemical Imaging Through Scattering Medium

***Shupeng Zhao*, Hilton B.de Aguiar**

Laboratoire Kastler Brossel, ENS-Université PSL, CNRS, Sorbonne Université, Collège de France. 24 rue Lhomond, 75005 Paris, France.

Imaging opaque biological specimens at-depth is a current challenge in optics as light passing through biological tissue experiences an environment of heterogeneous refractive index, leading to aberrations and scattering. Advanced fluorescence microscopy techniques—such as confocal and two-photon microscopy—enable deep imaging in turbid biological tissues by selectively detecting unscattered (ballistic) photons. However, beyond a depth of a few scattering mean free paths, this approach becomes ineffective, as ballistic photons are largely depleted. To address this limitation, feedback-based wavefront-shaping techniques have emerged as a powerful alternative. So far, wavefront shaping based imaging through scattering media has been successfully demonstrated in both two-photon and three-photon fluorescence modalities [1,2]. While previous attempts have been tried on Raman-based contrasts, they have been limited to invasive settings [3], the ballistic regime [4], or suffer from imaging speeds [5]. Here, we develop a non-invasive and fast wavefront shaping technique for coherent Raman microscope. We simultaneously modulate the wavefronts of the two excitation wavelengths using a sole spatial light modulator. Using such approach, we enable the retrieval of chemical information through scattering media through Raman spectroscopy. In this presentation, we will present our current results, outline key technical details, and discuss the differences and advantages of this method compared to previous methods.

References:

[1] Papadopoulos, Ioannis N., et al. "Scattering compensation by focus scanning holographic aberration probing (F-SHARP)." Nature Photonics 11.2 (2017): 116-123.

[2] Rauer, Bernhard, et al. "Scattering correcting wavefront shaping for three-photon microscopy." Optics Letters 47.23 (2022): 6233-6236.

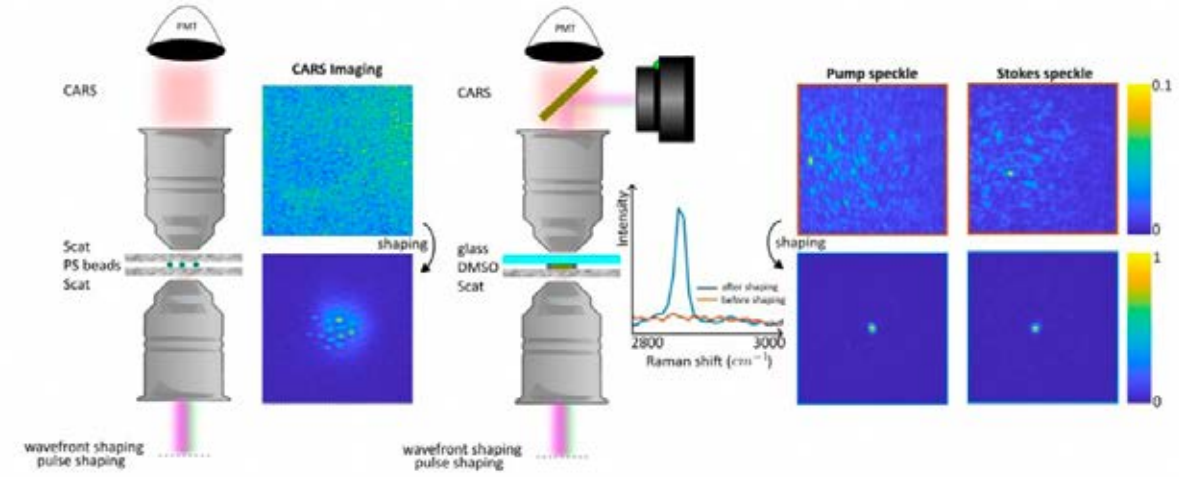
[3] Hofer, Matthias, et al. "Coherent anti-Stokes Raman scattering through thick biological tissues by single-wavefront shaping." Physical Review Applied 14.2 (2020): 024019.

[4] Wang, Weiqi, et al. "Polychromatic Adaptive Optics-Assisted Stimulated Raman Scattering Microscopy Enables Deep Tissue Chemical Imaging." Laser & Photonics Reviews 19.24 (2025): e01022.

[5] Tian, Bingxin, et al. "Non-invasive chemically selective energy delivery and focusing inside a scattering medium guided by Raman scattering." Optics Letters 47.9 (2022): 2145-2148.

Keywords: Coherent Raman, wavefront shaping, imaging through scattering medium

Fig.1



The setup and result of chemical imaging and spectroscopy through scattering medium.

Oral Abstracts

[Abstract:0500] [SERS/TERS/Plasmonics]

Direct Laser Written Periodic Nanostructures for Surface-Enhanced Raman Spectroscopy

***Ilayda Alparslan*, Serena Nur Erkızan, Fırat Idikut, Özge Demirtaş, Arian Goodarzi, Ahmet Kemal Demir, Mona Borra, Ihor Pavlov, Alpan Bek**

Physcis Department, Middle East Technical University, Ankara, Turkey

Surface-enhanced Raman spectroscopy (SERS) is a highly sensitive and nondestructive molecular detection technique that relies on amplification of the weak Raman scattering by electromagnetic field enhancement and/or the scattering cross-section enhancement and shows great promise across a wide range of fields, including biosensing, chemical detection, and single-molecule detection. However, it is limited by the need for reproducible, fast, and large-area fabrication. Femtosecond laser-induced periodic surface structures (LIPSS) provide a single-step, maskless, chemistry-free route to such substrates. Our group has previously demonstrated [1] that the fast fabrication of highly sensitive SERS substrates with large area and high uniformity for two different periodicity regimes: Low Spatial Frequency LIPSS (LSFL) and High Spatial Frequency LIPSS (HSFL) on crystalline silicon (Si). The SERS substrates deposited with silver (Ag) are found to be capable of detecting a Raman analyte down to 10^{11} M Crystal Violet (CV) molecules. Among the 532, 660, and 785 nm excitation wavelengths, both LSFL and HSFL Si surfaces are found to exhibit the strongest SERS under 660 nm excitation, exhibiting Raman enhancement factors (EFs) as high as 10^9. Raman enhancement factor simulations for all excitation wavelengths are performed using the Finite Element Method (FEM) based Maxwell solver. Enhancement factor results obtained from measured SERS spectra and electric-field enhancement simulations exhibit good agreement. Building on this foundation, here we present our detailed surface preparation studies for producing precisely tailored SERS substrates by varying LIPSS based fabrication parameters.

References:

[1] S. N. Erkızan, F. Idikut, Ö. Demirtaş, A. Goodarzi, A. K. Demir, M. Borra, I. Pavlov, A. Bek, LIPSS for SERS: Metal Coated Direct Laser Written Periodic Nanostructures for Surface Enhanced Raman Spectroscopy. Adv. Optical Mater. 2022, 10, 2200233. https://doi.org/10.1002/adom.202200233

Keywords: surface enhanced Raman spectroscopy, laser-induced periodic surface structures, high spatial frequency LIPSS, low spatial frequency LIPSS

[Abstract:0501] [Non-linear/Time-resolved]

Probing Microscopic Network Structure in Ultrathin Amorphous Layers by Time-Frequency Hybrid Coherent Raman Spectroscopy

***Ryu Yoshizawa*[1], *Keisuke Seto*[2], *Tsuneto Kanai*[2], *Atsunori Sakurai*[2], *Toshiki Sugimoto*[2]**

[1]*Graduate Institute for Advanced Studies, SOKENDAI, Okazaki, Aichi, 444-8585, Japan*
[2]*Department of Materials Molecular Science, Institute for Molecular Science, Okazaki, Aichi, 444-8585, Japan*

Nanometer-scale amorphous layers play important roles in a wide range of applications. In surface-activated bonding, direct bonding between crystals near room temperature is enabled through an ultrathin amorphous layer formed by atomic-beam irradiation of crystal surfaces. Although this layer is regarded as an essential factor in bonding, the influence of its microscopic structure and quality remains poorly understood. Because the layer is extremely thin, typically less than 10 nm, and because amorphous structures are inherently difficult to analyze quantitatively, direct characterization is highly challenging. Conventional spontaneous Raman scattering lacks the sensitivity required for this purpose, while diffraction-based methods are not well suited for the quantitative analysis of non-periodic structures. To overcome these challenges, we employ time-frequency hybrid coherent Raman spectroscopy, which combines high-sensitivity detection with time-domain separation of spectrally congested amorphous responses.

In this study, we investigate amorphous layers formed on quartz using coherent anti-Stokes Raman scattering (CARS), a third-order nonlinear Raman process well suited for detecting weak vibrational signals. By applying a tunable time delay to the probe pulse relative to the pump and Stokes pulses, we suppress the short-lived non-resonant response. More importantly, this time-resolved scheme enables selective detection of resonant vibrational coherence by exploiting differences in vibrational dephasing dynamics, thereby separating overlapping spectral contributions. We focus on the Si–O–Si bending-mode region, which serves as a spectral fingerprint of medium-range order and ring-size distribution in the amorphous network. To remove spectral interference from the underlying crystalline quartz substrate, we apply a maximum-entropy-based linearization procedure to the complex nonlinear polarizability, enabling clearer recovery and interpretation of the amorphous response.

For demonstration, we prepared a series of z-cut quartz samples with amorphous surface layers about 10 nm thick by Ar-beam sputtering, systematically varying the irradiation time. By comparing the reconstructed amorphous responses, we tracked microscopic structural changes induced by different formation conditions. The combination of time-delayed nonlinear coherent Raman measurements and maximum entropy analysis allowed us to isolate the amorphous-layer response and identify structural differences among the samples. These results demonstrate the utility of time-frequency hybrid coherent Raman spectroscopy for quantitative characterization of ultrathin amorphous layers.

Keywords: coherent Raman spectroscopy, time-resolved spectroscopy, amorphous network structure, thinfilm material, solid interfaces

[Abstract:0508] [SERS/TERS/Plasmonics]

Microplasma-Enabled Nanoheterostructures for SERS Detection of Aβ Oligomers in Alzheimer's Diagnosis

***Yen Ling Chiu*, Wei Hung Chiang**

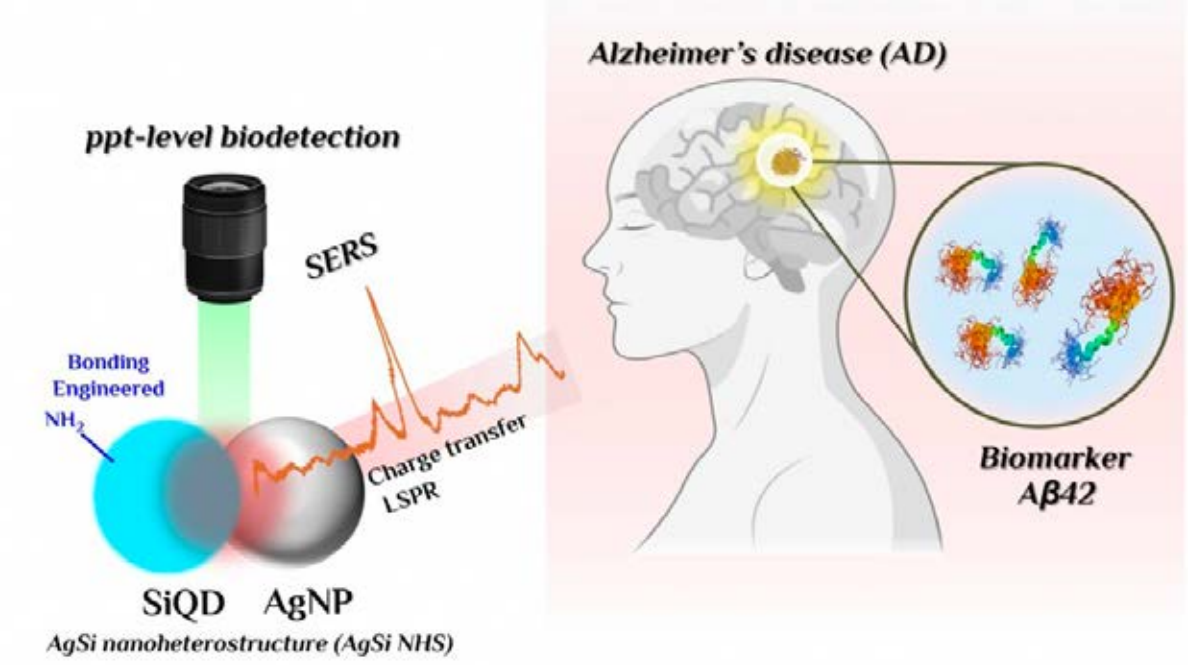
Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei City, Taiwan

Alzheimer's disease (AD), a neurodegenerative disorder affecting over 50 million people worldwide and projected to rise to 135 million by 2050, is characterized by memory loss and cognitive decline. Its pathology begins with the accumulation of amyloid-β (Aβ) and the spread of tau pathology. Among Aβ forms, oligomers are highly cytotoxic and strongly linked to cognitive deficits. The prolonged gap between amyloid fibrillogenesis and symptom onset underscores the importance of early diagnosis by detecting Aβ oligomers, enabling timely therapeutic interventions to mitigate cognitive decline.

Surface-Enhanced Raman Spectroscopy (SERS) is a powerful technique for detecting AD biomarkers like Aβ42 oligomers at ultra-low concentrations. Compared to conventional methods like enzyme-linked immunosorbent assay (ELISA), SERS provides higher sensitivity, better resolution, cost-efficiency, and enables label-free analysis for detailed protein structure investigation. In the application of SERS, the choice of a suitable SERS-active substrate is critical. In our work, silicon quantum dot-silver nanoparticle nanoheterostructures (SiAgNHS) is a promising metal-semiconductor hybrid system that combines localized surface plasmon resonance (LSPR) and charge transfer (CT) effects for enhanced Raman sensitivity. Fabricated via a controllable and scalable microplasma technique under ambient conditions, SiAgNHS eliminates the need for high temperatures, strong acids, and vacuum systems, making the process environmentally friendly.8 In the TEM figure, the obvious bonding between SiQD and AgNPs was observed confirming the successful design of the SERS biosensor. The SiAgNHS exhibits tunable plasmonic coupling, leading to superior Raman enhancement properties. Importantly, SiAgNHS has demonstrated the ability to differentiate between Aβ42 monomers and oligomers, both of which are critical for understanding the early pathological mechanisms of AD. This biosensor achieved a detection limit of 1 pM for both Aβ42 monomers and oligomers, showcasing exceptional sensitivity and reliability. This detection limit is lower than the disease concentrations of Aβ42 oligomers typically found in human CSF and blood which are 0.57 nM and 15 pM respectively. This advancement provides a powerful tool for early diagnosis of AD and highlights the potential of SiAgNHS in developing efficient and accessible diagnostic methods.

Keywords: Alzheimer's disease, biosensor, microplasma

AgSi Nanostructures for SERS Detection of Aβ42



[Abstract:0511] [Materials]

Dual Role of Raman Spectroscopy in Nanosensor Fabrication: Monitoring and Laser Processing of Carbon Nanotubes

***Miroslav Haluska**, Ines Kraiem, Cosmin Ioan Roman, Nicolas Monnerat, Jan Puntschart, Juliano Aebi, Pengcheng Zhang, Christofer Hierold.*

Micro and Nanosystems, Department of Mechanical and Process Engineering, ETH Zürich, Switzerland

Carbon nanotubes (CNTs) are promising materials for nanoscale electronic devices, including gas sensors; however, their practical implementation requires reliable synthesis, precise localization, and controlled integration of individual nanotubes into functional device architectures. In this work, Raman spectroscopy is presented as a versatile and indispensable tool in the fabrication of CNT-based nanosensors, serving both as a characterization and a processing technique.

First, Raman spectroscopy is employed as a non-destructive monitoring tool during CNT synthesis and device fabrication. It enables evaluation of key nanotube properties such as diameter, structural quality, and electronic type through analysis of the radial breathing mode (RBM), as well as the D and G bands, including their positions, intensities, and line shapes. Raman mapping is utilized for localization of individual suspended CNTs grown by chemical vapor deposition (CVD) in a CH_4/H_2 atmosphere using ferritin-based Fe catalyst precursors [1], and for selecting suitable nanotubes for integration into carbon-nanotube field-effect transistor (CNTFET).

The efficiency of Raman spectroscopy for visualization of suspended CNTs was systematically evaluated and compared with scanning electron microscopy (SEM). Multi-wavelength Raman measurements using 488 nm and 514 nm excitation lasers achieved a combined detection yield approaching 96%, demonstrating the high reliability of Raman spectroscopy for nanotube localization and highlighting the resonance effect impact [2].

Second, the Raman excitation laser can act as a localized processing tool, enabling modification of CNTs. Laser-induced effects such as removal of surface contamination, defect formation, oxidation, and structural modification can be exploited to influence nanotube properties and device performance.

These results demonstrate that Raman spectroscopy is not only a powerful characterization method but also an enabling tool for monitoring, controlling, and improving the fabrication of CNT-based nanosensors.

References:

[1] L. Durrer et al., Nanotechnology, 20 (2009) 355601.

[2] N. Monnerat et al., J. Sens. Sens. Syst., 14 (2025) 67–73.

Keywords: carbon nanotubes, Raman spectroscopy, nanodevices

[Abstract:0512] [Coherent Raman Imaging]

Feature Level Validation of Label-Free Intraoperative Histology in Glioblastoma Using Stimulated Raman Scattering İmaging

***Max Brinkmann*[1], *Silke Morris*[1], *Felix Neumann*[1], *Ramon Droop*[1], *Steffen Ullmann*[1], *Tim Hellwig*[1], *Felix Stark*[2], *Christoph Sippl*[2], *Stefan Linsler*[2], *Jürgen Schnekenburger*[3]**

[1]*Refined Laser Systems GmbH, Mendelstraße 11, 48149 Münster, Germany*
[2]*Department of Neurosurgery, Medical Campus Oberfranken, Bayreuth, Germany*
[3]*Biomedical Technology Center, University of Münster, Mendelstraße 17, 48149 Münster, Germany*

Stimulated Raman Scattering (SRS) imaging has emerged as a powerful modality for rapid, label-free histopathological assessment of biological tissues. While previous studies primarily compared SRS with conventional histology at the level of overall diagnostic classification, feature level validation is required to determine whether established diagnostic histopathological features can be reliably identified from label-free SRS contrast.

Here we investigate feature level validation of SRS based histology using a mobile SRS imaging platform designed for intraoperative use, enabling real-time analysis of specimens directly within the operating room. The system provides access to both the CH-stretch region for structural imaging and the fingerprint region for biochemical characterization with microsecond pixel dwell times suitable for rapid intraoperative imaging.

We evaluated the clinical applicability of SRS imaging in a cohort of 30 human glioblastoma samples. Each specimen was divided into two portions, with one portion examined by SRS imaging without sectioning and the other processed for conventional histopathology. First, virtual hematoxylin and eosin images generated from SRS data were compared to conventional histology in a blinded study involving ten pathologists without prior experience in SRS image interpretation. The pathologists assessed diagnostically relevant features including hypercellularity, cellular and nuclear pleomorphism, hypervascularization, endothelial proliferation, mitotic activity, necrosis, and pseudopalisading. All features except mitotic activity were identified with comparable detection rates in SRS images and conventional histology, supporting the reliable interpretation of SRS derived histology.

Second, we explored the diagnostic potential of hyperspectral SRS data from the fingerprint region. Spectral datasets were analyzed using non-linear dimensionality reduction. Preliminary results indicate that intrinsic molecular signatures captured by SRS enable discrimination of MGMT promoter methylation status, with approximately 80% of samples clustering according to their molecular profile. As MGMT promoter methylation is associated with response to alkylating chemotherapy, these findings support the potential of SRS imaging for rapid assessment of molecular tumor characteristics.

Keywords: SRS, Histology, Intraoperative, Label-free

[Abstract:0516] [SERS/TERS/Plasmonics]

Improving SERS Sensitivity Using Metal Nanoparticles in Textured Silicon Cavities

***Zeynep Cantürk*, Ghazanfar Ali Khan, Alpan Bek**

Department of Physics, Middle East Technical University, 06800, Ankara, Türkiye

Raman spectroscopy is widely used in many fields to identify molecules or materials such as pollution monitoring, narcotics detection, food safety analysis. Because Raman spectroscopy conventionally produces inherently weak signals, surface enhancement techniques are employed to detect sensitivity, which are called surface enhancement Raman spectroscopy (SERS). Over the past decades many strategies have been developed to improve SERS substrates and to increase Raman enhancement factors. One of these approaches is surface texturing through various etching processes while the other one is using metal nanoparticles like silver or gold to generate plasmonic resonance with these particles.

In this study, we aim to fabricate SERS substrates by using photochemical etching method and metal assisted photochemical etching. In addition, the deposition of metal nanoparticles is studied with different shapes and sizes onto these cavity surfaces, Raman measurements is investigated using crystal violet (CV) as the analyte at 532 nm and 785 nm wavelength. Because of the increasing the plasmonic enhancement (metal-based) provided by MNPs, a significant improvement in the EF is observed compared to only textured substrates. Furthermore, FDTD simulations indicate that placing MNPs inside the cavities of SERS substrates increases the EF from 10^4 to 10^7 across the visible wavelength range (300–800 nm).

Keywords: surface-enhanced Raman scattering, MNPs on the Texturing Surface, Photochemical Etching

Oral Abstracts

[Abstract:0524] [Coherent Raman Imaging]

Multimodal High-Speed Laser-Scanning Submicron Infrared (O-PTIR) and Stimulated Raman (PT-SRS) Platform for Real-Time Label-Free Chemical Imaging

***Mustafa Kansiz*, Yuhao Yuan, Carolin Borbeck, Miriam Unger**

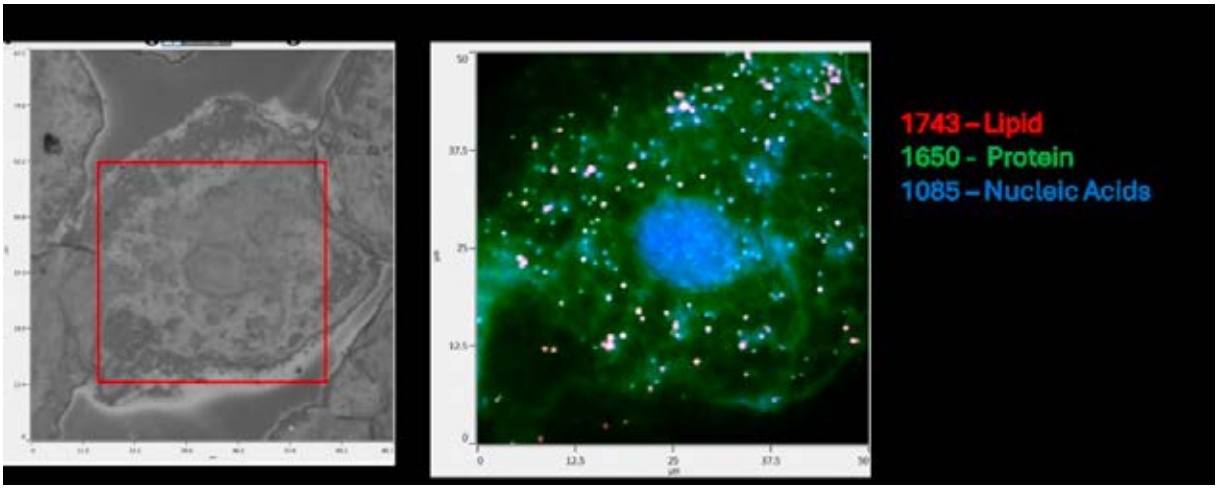
Photothermal Spectroscopy Corp

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

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

Keywords: Infrared spectroscopy, Raman, Stimulated Raman, Photothermal, multimodal, fluorescence

Cheek cell with laser scanning OPTIR



high Speed, high resolution sub-500nm imaging of a cheek cell in seconds

[Abstract:0601] [Biology/Biomedicine]

Navigating Complex Biological Platforms: From Nanobiosensors to Bioimaging

Deniz Yılmaz

Department of Genetics and Bioengineering, Yeditepe University, Istanbul, Türkiye

Raman spectroscopy is a powerful vibrational spectroscopic technique that provides high selectivity and sensitivity across diverse fields, ranging from material characterization to pharmaceuticals. In recent years, its importance in biological applications has grown significantly, largely due to its unique ability to analyze liquid samples without water interference.

In our research, we utilize the WITec alpha300 R confocal Raman system, which offers versatile capabilities tailored to our analytical needs. For biological applications, the setup features an adaptable inverted microscope architecture equipped with top-down and bottom-up illumination options. This capability is crucial for non-invasive measurements of biological samples directly within buffers or cell culture media.

Our work primarily focuses on biotechnology, categorized into two main areas: nanobiosensor development and bioimaging. For nanobiosensor applications, we focus on developing Surface-Enhanced Raman Scattering (SERS)-based platforms for bacterial detection at low limits of detection (LOD). Here, the WITec system achieves high sensitivity owing to its high spatial resolution and small confocal volume, which effectively suppresses background interference and enhances the signal-to-noise ratio.

For bioimaging, the system enables label-free chemical mapping of cellular and tissue samples. Utilizing high spatial resolution combined with integrated TrueSurface technology, we capture simultaneous topographical and Raman images across complex surfaces, such as blood cells, tissues, and biological structures like diatoms, without requiring extensive sample preparation or chemical labeling.

In summary, the spatial resolution, optical flexibility, and integrated TrueSurface capabilities of the WITec system significantly streamline our workflow. This combination enables the development of sensitive SERS nanobiosensors and supports reliable label-free bioimaging.

Keywords: Navigating, Complex Biological Platforms, Nanobiosensors, Bioimaging

[Abstract:0602] [Biology/Biomedicine]

Misclassification-Driven Insights into Abnormal Changes in the Hamster Buccal Pouch: A Serum Raman Spectroscopy Approach

***Sampurno Banerjee*[1,2], *Abhinendra Kumar*[1], *Arti Hole*[1], *Arvind Ingle*[1], *Arvind Ingle*[2], *Murali Krishna*[1], *Murali Krishna*[2]**

[1]*Chilakapati Lab, ACTREC-TMC, Kharghar, Navi Mumbai, Maharashtra, India*
[2]*Homi Bhabha National Institute, Anushakti Nagar, Maharashtra, India*

Oral carcinogenesis is a multistep process, and early diagnosis remains critical for improving patient outcomes. Biopsy and histopathology, the current gold standards, are invasive and impractical for mass screening or remote diagnosis. Because clinically normal-looking tissue can still harbor underlying biochemical changes due to field cancerization, early detection remains a persistent challenge. Serum Raman spectroscopy (RS) offers a minimally invasive way to pick up on these subtle biochemical shifts before they become clinically apparent. In this study, we used the hamster buccal pouch (HBP) model, with cancer induced through topical application of 0.5% DMBA, to explore this further.

Serum spectra were acquired weekly over 14 weeks from DMBA-treated (T), vehicle control (V), and untreated control (C) animals across two independent batches, using a WITec alpha300R Raman confocal microscope (532 nm laser, ~30 mW power, 5s integration, 10 accumulations). Spectra were analyzed using PCA and supervised PC-LDA. A substantial proportion of control and vehicle animals were misclassified as tumor-bearing during later stages of the carcinogenesis period.

To understand this misclassification during the later weeks, animals were re-categorized and pooled (9–11 and 12–14 week) into four groups: Controls (C), Flagged (F; controls misclassified more than twice), True Classified (TC; correctly identified tumors), and Misclassified (MC; tumors misclassified as control). F and TC clustered more closely with each other than with C and MC, and vice versa — pointing to two distinct, independently acting confounders. Chronic injury-driven protein elevation appears to link F and TC, while lipemia-driven lipid elevation links C and MC, supported by MCR-ALS data showing elevated lipid signatures in MC sera. Both mechanisms align with existing literature on chronic mechanical irritation and metabolic shifts in carcinogenesis models.

Both batches exhibited a trend for increased classification corresponding to the histological progression of hyperplasia, dysplasia and squamous cell carcinoma. These results corroborate the evidence that RS can be used to detect abnormal alterations in normal appearing samples, thereby validating previous tissue-based findings and suggesting that RS could be a useful minimally invasive screening tool for early detection of oral cancer and risk stratification in field cancerization-affected clinical settings.

Keywords: Misclassification-Driven Insights, Abnormal Change, Hamster Buccal Pouch, A Serum Raman Spectroscopy Approach

[Abstract:0603] [Biology/Biomedicine]

Revealing Label-Free, Multiplexed Molecular İnformation For Mechanobiology Through Raman Spectroscopy And Advanced Data Science

Monica Marro

Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza and CIBER-BBN, Zaragoza, Spain
Fundación Agencia Aragonesa para la Investigación y el Desarrollo (ARAID), Zaragoza, Spain

Mechanobiology has developed sophisticated approaches to apply and quantify mechanical forces in living systems. However, methods capable of simultaneously revealing the molecular response of cells to mechanical perturbation without exogenous labels remain scarce. We envision that the combination of Raman spectroscopy with advanced chemometric and data science approaches can bridge this gap by transforming complex vibrational spectra into biologically meaningful molecular information.

Here, we present the evolution of a research line aimed at establishing Raman spectroscopy as a label-free and multiplexed molecular readout for mechanobiology. This work began with the integration of Raman spectroscopy and optical tweezers to simultaneously manipulate and probe biological samples, demonstrating the feasibility of monitoring force-induced molecular changes in DNA molecules and red blood cells. In parallel, we developed advanced chemometric and data science methods to identify molecular signatures associated with mechanically induced cellular responses from complex Raman datasets.

Building on this foundation, we applied this approach to investigate the molecular response of living cells under mechanical confinement, revealing that cPLA2 activity at the inner nuclear membrane produces arachidonic acid, which is a metabolite regulating cortical contractility in confinement [1] (in collaboration with V. Ruprecht, S. Wieser and V. Venturini). Importantly, these findings demonstrated that label-free Raman spectroscopy can identify biochemical pathways activated by mechanical stress in living cells.

We are currently extending this framework to cancer mechanobiology by developing label-free Raman imaging strategies to study cancer cells migrating through highly confined microfluidic channels and cancer organoids (in collaboration with M2BE group in University of Zaragoza). By integrating molecular imaging with advanced computational analysis, we aim to uncover molecular programs associated with confinement, invasion and mechanotransduction in physiologically relevant models.

Together, these advances establish Raman spectroscopy not simply as a molecular imaging technique, but as a functional molecular readout of cellular mechanotransduction. These studies lay the foundations for a next-generation mechanobiology platform that integrates mechanical perturbation, label-free Raman spectroscopy and advanced data science methods to decode mechanotransduction across biological systems, from single biomolecules to cancer organoids.

Reference:

[1] Venturini V., et al, Science 2020

POSTERS

[Abstract:0012] [Novel Approaches]

Development of Broadband Multiplex Coherent Anti-Stokes Hyper-Raman Scattering (CAHRS) Spectroscopy

***Kazuki Inoue*, Masanari Okuno**

Department of Basic Science, The University of Tokyo, Meguro, Tokyo, Japan

We recently developed coherent anti-Stokes hyper-Raman scattering (CAHRS) spectroscopy, which provides information on hyper-Raman (HR) resonances at high speed [*Nat. Commun.* 2025, 16, 306]. Expanding the applications of CAHRS spectroscopy to diverse fields, including imaging and ultrafast spectroscopy, requires several instrumental improvements. In this study, we successfully broadened the spectral window of the CAHRS experimental setup, enabling simultaneous spectral acquisition across the fingerprint region by employing a white-light continuum as a Stokes beam.

Figure 1 shows the diagram of the CAHRS process. In the CAHRS process, ω_1 and ω_2 pulses excite the vibrational coherences with a frequency of $\Omega=2\omega_1-\omega_2$. Then, an additional ω_1 pulse induces a fifth-order nonlinear polarization with a frequency of $4\omega_1-\omega_2$, which emits CAHRS signals.

Figure 2 shows our broadband multiplex CAHRS spectrometer. A femtosecond Yb: KGW laser was used to generate both narrowband ω_1 (wavelength: 1030 nm, pulse energy: ~ 2.5 μJ/pulse, repetition rate: 10 kHz) and broadband ω_2 (515 ~ 750 nm corresponding to $2\omega_1-\omega_2$ = 0 ~ 6000 cm^{-1}, sub-ps, ~ 4 nJ/pulse) beams. The broadband ω_2 light was obtained by a white-light generation in a sapphire plate. Two beams were focused on the samples at angles satisfying the phase-matching condition. The exposure time was 10 s, and 20 exposures were averaged. It should be emphasized that the spectral range of the present CAHRS setup is determined by the ω_2 light, whose spectral profile, shown in Figure 3, spans the entire spectral region.

Figure 4 shows a CAHRS spectrum of a 1 mM *all-trans* retinal chloroform solution from 500 to 2000 cm^{-1}. The spectrum was normalized by that of neat chloroform as a non-resonant background. It is clear that the CAHRS spectrum contains multiple vibrational resonances over the range from 700 to 1700 cm^{-1}. The largest dispersive band around 1580 cm^{-1} is attributed to the C=C stretching mode of all-trans retinal. Our result suggests that our broadband multiplex CAHRS spectrometer can simultaneously detect molecular vibrations across the fingerprint region. By combining with the maximum entropy method (MEM), we have successfully retrieved vibrationally resonant components from 500 to 2000 cm^{-1}.

Keywords: hyper-Raman spectroscopy, coherent anti-Stokes hyper-Raman scattering spectroscopy, coherent Raman spectroscopy, nonlinear spectroscopy

Figure 1 Diagrams of spontaneous HR and CAHRS processes.

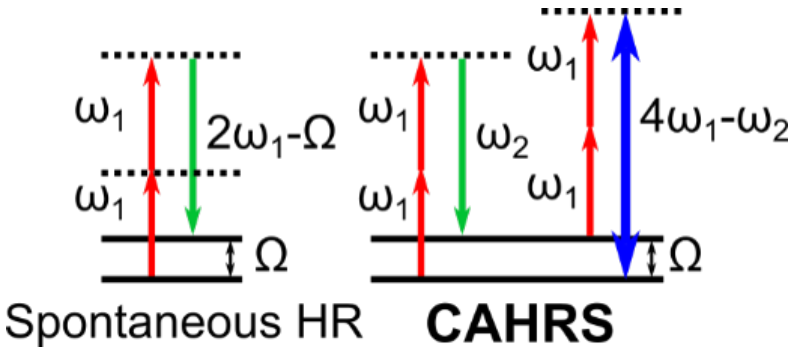


Figure 2 Broadband multiplex CAHRS spectrometer.

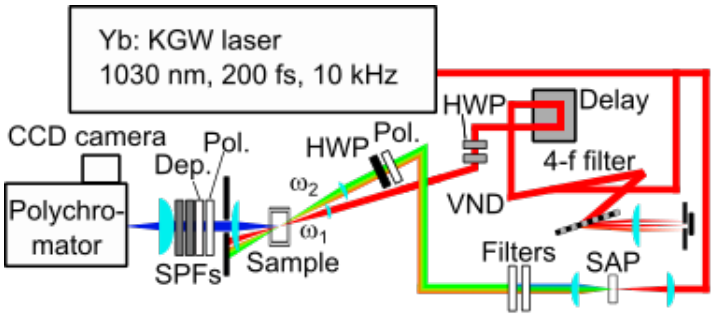


Figure 3 A spectral profile of the ω_2 light.

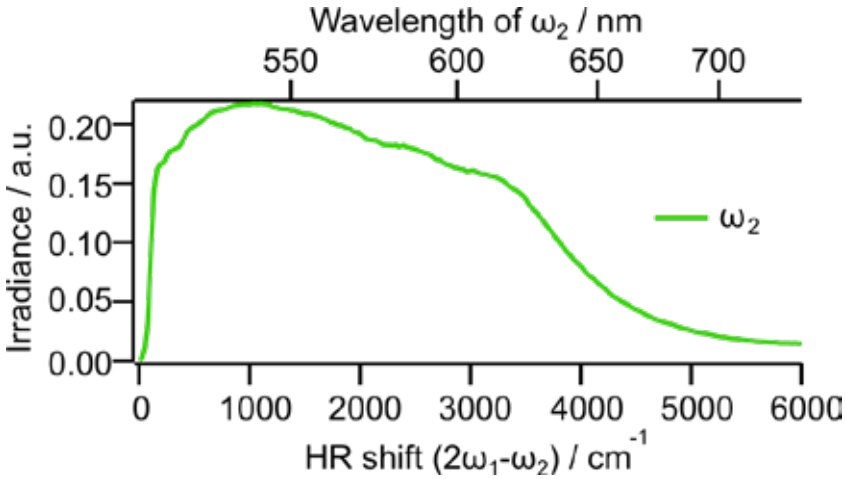
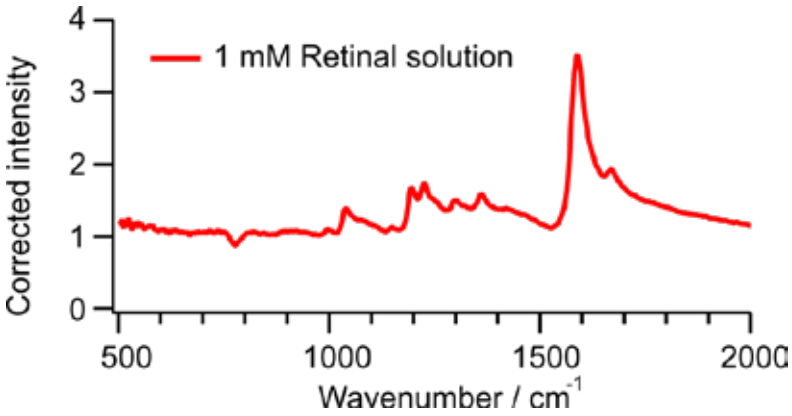


Figure 4 CAHRS spectrum of 1 mM retinal solution.



[Abstract:0023] [Materials]

Evaluation of Spatially Offset Raman Spectroscopy For Depth-Selective Analysis of Highly Scattering (Layered) Paint Systems in Cultural Heritage

***Merel C. Konings*[1], *Franca Van Diederen*[1], *Freek Ariese*[2], *Matz Liebel*[1], *Maarten R. van Bommel*[3], *Govert W. Somsen*[4]**

[1]*Department of Physics and Astronomy, Vrije Universiteit Amsterdam, De Boelelaan 1100, Amsterdam 1081 HZ, The Netherlands*
[2]*Department of Physics and Astronomy, Vrije Universiteit Amsterdam, De Boelelaan 1100, Amsterdam 1081 HZ, The Netherlands, Deceased*
[3]*Van 't Hoff Institute for Molecular Sciences, Faculty of Science, University of Amsterdam, Science Park 904, 1098 XH, Amsterdam, Netherlands*
[4]*Division of bioanalytical Chemistry, Amsterdam Institute for Molecular and Life Sciences, Vrije Universiteit Amsterdam, De Boelelaan 1085, Amsterdam 1081 HV, The Netherlands*

Photodegradation can cause progressive chemical breakdown of molecules in many materials, thereby altering their appearance and performance. Understanding the chemistry of light-induced degradation (LID) is highly challenging due to the complexity of the, often heterogeneous, materials investigated and the many environmental aspects that play a role. Rational control and prevention of LID is only possible with a thorough understanding of the chemical processes involved, which requires the availability of accurate and quantitative analytical tools to identify and quantify the composition of light-degraded samples under relevant conditions.

In this work, we investigate the potential of spatially offset Raman spectroscopy (SORS) for the selective, non-invasive analysis of solid materials, with particular focus on analysis of surface and subsurface levels. Within a cultural heritage context, a series of polydimethylsiloxane (PDMS) and paint mock-ups with systematically controlled properties (e.g., scattering behavior, layer thickness, and absorption coefficients) were developed to evaluate the potential of SORS for the identification of pigments and dyes in layered paint systems and different binding media. The influence of these material parameters on the effective penetration depth and spectral selectivity is discussed. Our results demonstrate that SORS can provide an effective means for probing subsurface chemical changes, thereby offering opportunities for the selective, non-invasive analysis of light-exposed solid materials. This will contribute to an improved understanding of photodegradation pathways of colorants in works of art.

Keywords: Subsurface analysis, Spatially offset Raman spectroscopy, Cultural heritage

[Abstract:0025] [Coherent Raman Imaging]

Instrumentation for Super-Broadband Stimulated Raman Scattering Spectroscopy and Imaging

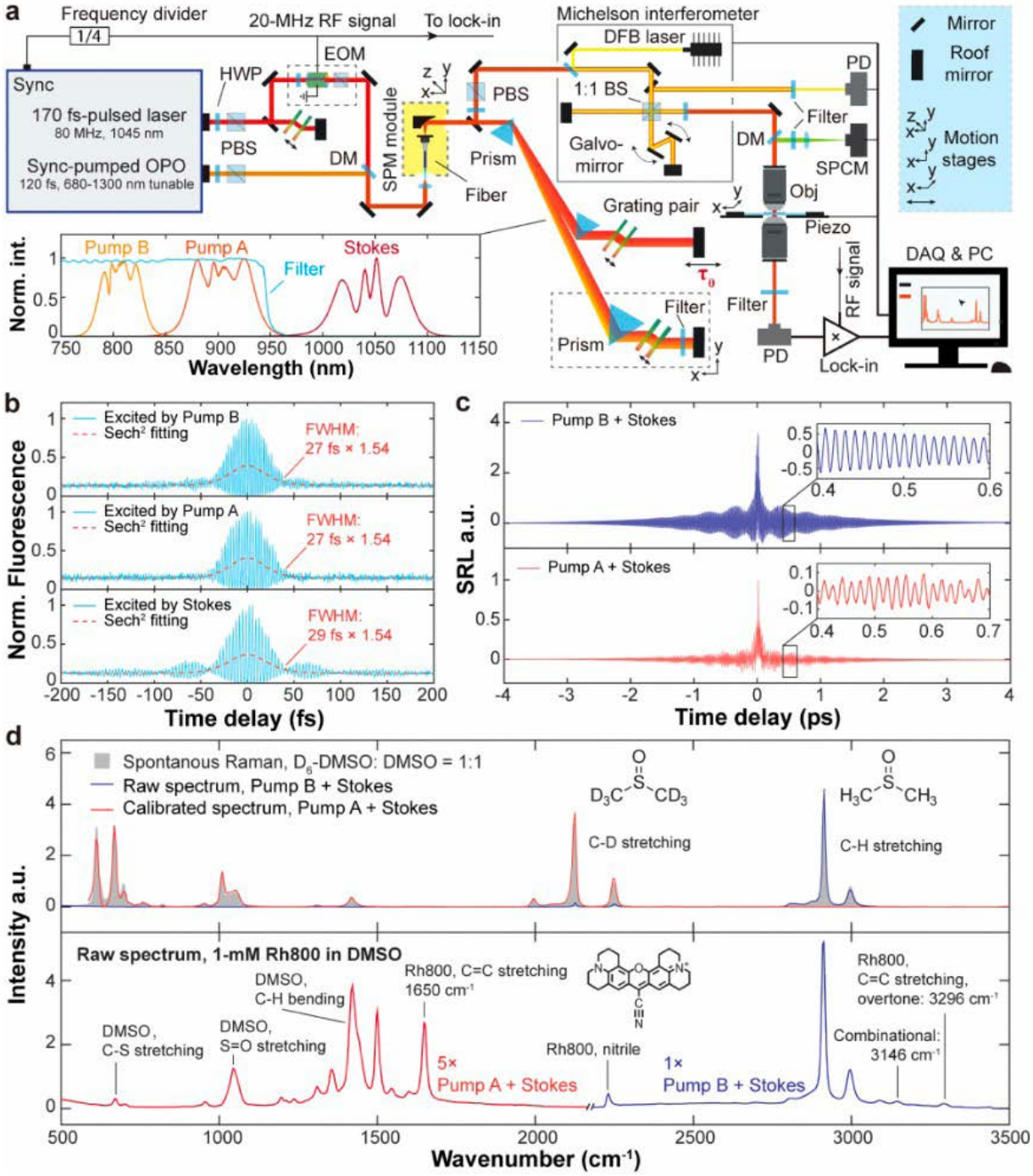
Jin Guo, Qiaozhi Yu, Haojie Zhang, Hanqing Xiong

National Biomedical Imaging Center, College of Future Technology, Peking University, Beijing, China.

Raman spectroscopy is a valuable tool widely used in biology and medicine. While still serving as the mainstream approach for high-fidelity Raman spectral analysis and imaging, spontaneous Raman scattering suffers from low acquisition speed and fluorescence interference. Here we report super-broadband stimulated Raman scattering (SuperB-SRS), a technique able to provide identical spectra to state-of-the-art spontaneous Raman over thousands of wavenumber ranges while being orders of magnitude faster and naturally supporting simultaneous multiplexed fluorescence detection. SuperB-SRS encodes the ideal Raman free induction decays into the stimulated Raman loss through few-cycle laser-induced quantum interference, permitting universal Raman analysis and imaging that unites high spectral fidelity, natural-linewidth-limited spectral resolution, broad bandwidth and state-of-the-art sensitivity. We demonstrate more than a 100-fold increase in speed for imaging of biological tissue samples compared with spontaneous Raman. As a medical application, we detect in clinical serum samples 11 biomarkers widely used to assess liver and kidney functions, cardiovascular diseases and other conditions. SuperB-SRS thus enables generating high-quality, large-scale datasets for data-driven health science, promising wide applications in multiple fields of science.

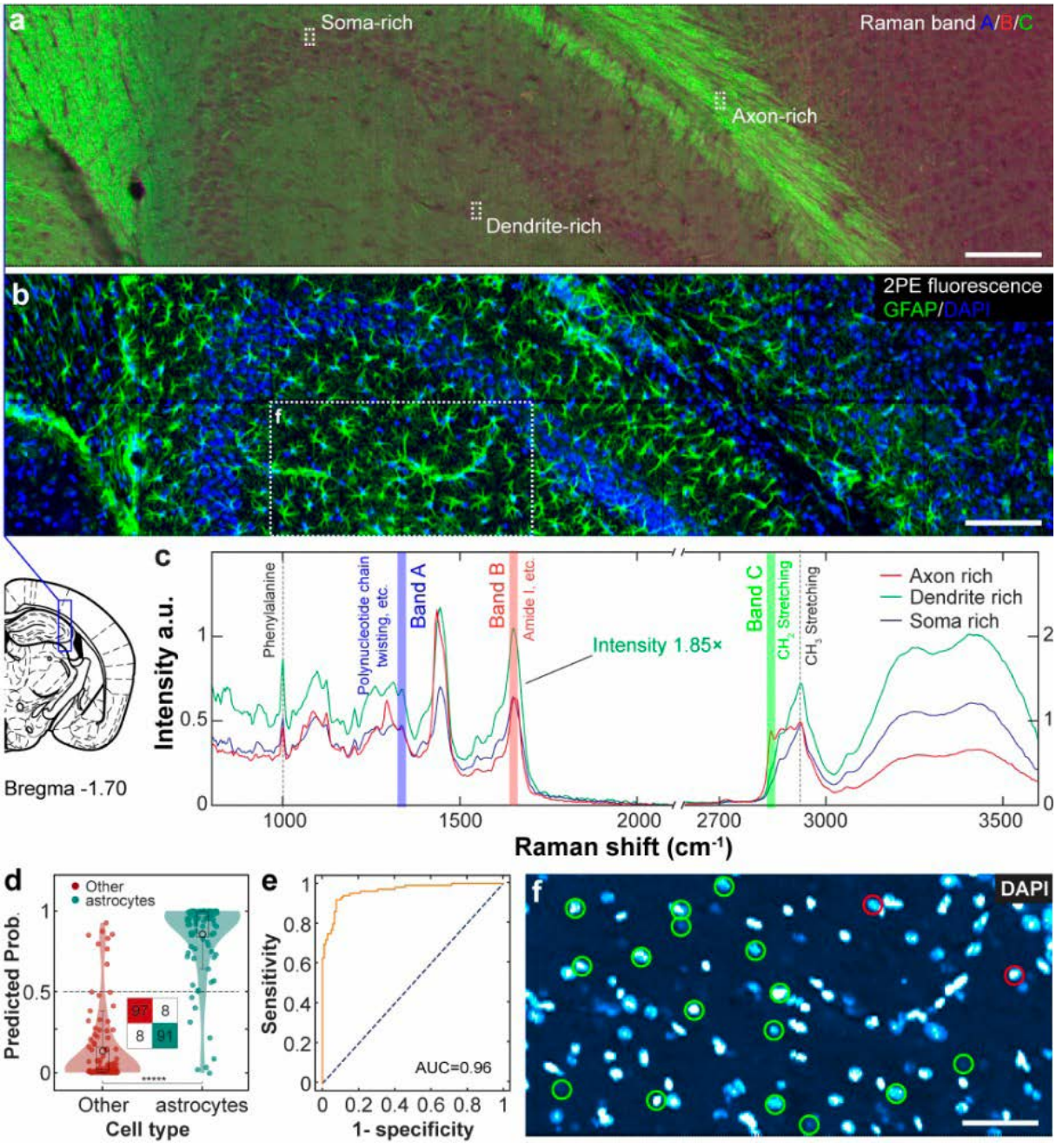
Keywords: Super-broadband, SRS, time-domain

SuperB-SRS spectroscopy



SuperB-SRS spectroscopy setup and full-range Raman spectra of typical molecules

Multimodal imaging of the brain tissue



Multimodal Imaging of Brain Tissue Integrating SuperB-SRS and Two-Photon Fluorescence

[Abstract:0038] [SERS/TERS/Plasmonics]

Raman Imaging as a Tool for Evaluating Drug Distribution in Starch-based Orodispersible Films

***Francesca Lovati*[1], *Helena Isabel Seguro Nogueira*[2], *Alois Bonifacio*[1], *Tito Trindade*[2]**

[1]*Department of Engineering and Architecture, University of Trieste, Trieste, Italy*
[2]*Department of Chemistry and CICECO- Aveiro Materials Institute, University of Aveiro, Aveiro, Portugal*

The use of orodispersible films (ODFs) has emerged in recent years as a strategy to overcome several limitations of conventional pharmaceutical dosage forms, particularly for pediatric and geriatric patients who experience difficulties in swallowing. In these solid pharmaceutical forms, achieving a homogeneous distribution of the active pharmaceutical ingredient (API) within the solid matrix is crucial, although it can often be challenging to assess. The aim of this study was to investigate the applicability of Raman spectroscopy and confocal Raman microscopy for assessing drug content distribution in these pharmaceuticals. As such, Raman studies were carried out on starch-based ODFs prepared by a simple solvent casting method, using sodium diclofenac (DCF) as a model drug. DCF is a well-known representative of nonsteroidal anti-inflammatory drugs (NSAIDs) and it is also used in infants, children, and adolescents worldwide.

It is well known that conventional Raman spectroscopy presents limitations for monitoring APIs at very low concentration in pharmaceutical formulations. Indeed, our results have demonstrated that conventional Raman spectroscopy was no longer able to detect DCF at a concentration of 0.1 wt% in the ODFs. Consequently, at these low concentrations, starch based ODFs were synthesized with the addition of gold nanoparticles (Au NPs), which act as plasmonic metallic Surface-enhanced Raman spectroscopy (SERS) substrates, enabling the identification of DCF down to 0.05 wt%. Raman and SERS imaging studies were also performed to evaluate the spatial distribution of DCF within the polymeric matrix. Finally, SERS studies were carried out on samples after depositing Au NPs onto the ODFs to simulate a real-use analytical scenario; also in this case, the lowest detectable concentration was 0.05 wt%. These results indicate that Raman and SERS imaging are alternative techniques for evaluating the distribution of APIs within starch-based ODFs, while also offering the advantage of detecting the drug at very low concentrations.

Keywords: Surface-enhanced Raman scattering (SERS), Gold nanoparticles, Raman imaging, Pharmaceutical detection

[Abstract:0040] [SERS/TERS/Plasmonics]

Surface-Enhanced Raman Spectroscopy for Detecting Microplastic-Induced Biochemical Changes in Vigna Radiata Leaves

***Hongshu Pu*, Yunfeng Li, Javier Plou, Andreas Seifert**

CIC nanoGUNE, San Sebastián, Spain

Microplastic contamination is increasingly recognized as a stress factor in terrestrial ecosystems, yet sensitive detection of early biochemical responses in plants remains challenging. While physiological parameters provide general information on plant status, molecular-level analytical methods may offer additional insight into subtle stress-induced alterations. Surface-enhanced Raman spectroscopy (SERS) enables label-free characterization of biochemical composition and is well suited for probing such changes.

In this study, SERS was applied to investigate biochemical variations in *Vigna radiata* leaves exposed to polystyrene microplastic particles. Leaf extracts from control and treated plants were deposited onto PDMS/AgNP substrates for spectral acquisition. A structured quality control workflow was implemented, including controlled substrate preparation, assessment of batch reproducibility, standardized sample handling, and multiple spatial measurements per sample to account for intrinsic heterogeneity and ensure spectral consistency.

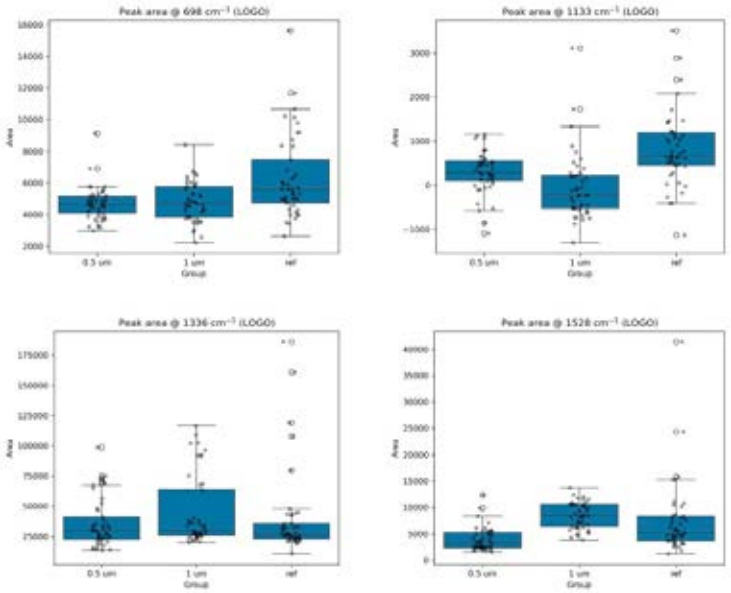
Systematic intensity differences were observed within the 1000–1650 cm^{-1} region, particularly in bands associated with aromatic ring vibrations, C=C stretching modes, and metabolite-related features. These spectral variations were reproducible across biological replicates and treatment groups, indicating exposure-related modulation of leaf biochemical composition. Under the same conditions, chlorophyll a and b measurements exhibited moderate and consistent variations among groups, supporting the presence of coordinated biochemical and physiological responses.

Preprocessed SERS spectra were analyzed using principal component analysis to explore variance structure, followed by supervised classification to assess group separation. Variable selection identified Raman regions contributing most strongly to differentiation between control and microplastic-treated samples.

The results show that SERS provides reproducible information on molecular level associated with microplastic exposure and supports its use for monitoring stress-related biochemical changes in plant systems.

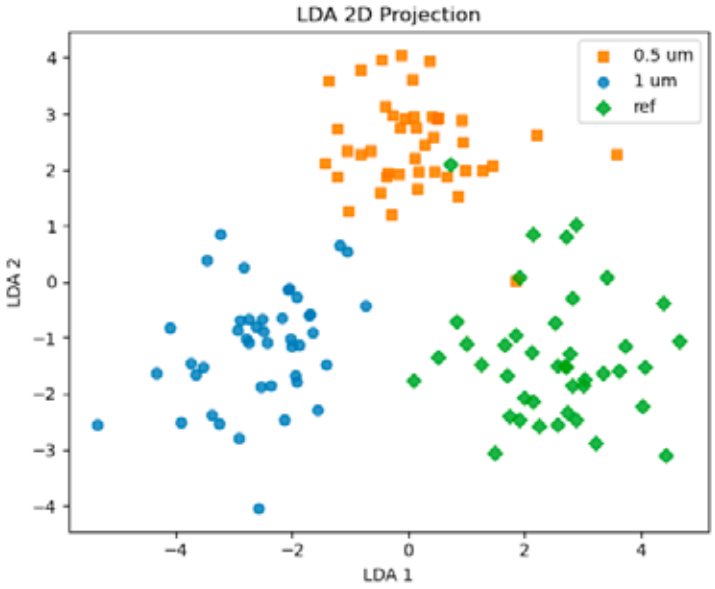
Keywords: Surface-enhanced Raman spectroscopy, Microplastics, Plant biochemical response, Vigna radiata, Mung bean

4 Key Peaks Group Comparison.png



Boxplot comparison of peak areas at the four selected Raman bands (698, 1133, 1336, and 1528 cm^{-1}) across control (ref) and microplastic-treated groups (0.5 μm and 1 μm). These bands were identified through systematic feature selection as the most discriminative spectral regions contributing to group differentiation. The minimal 4-peak model was evaluated using leave-one-group-out cross-validation (LOGO), achieving a classification accuracy of 0.74 ± 0.24 across 135 spectra. A permutation test ($p = 0.005$) further supported the statistical robustness of the model. The distributions illustrate consistent, group-dependent variations in spectral intensity associated with microplastic exposure.

LDA Group Separation



Two-dimensional projection of SERS spectra using linear discriminant analysis (LDA) to evaluate group separation between control (ref) and microplastic-treated samples (0.5 μm and 1 μm). The projection illustrates distinct clustering patterns among groups, indicating that exposure-related spectral differences contain sufficient discriminative information for classification. This result supports the presence of systematic biochemical variations associated with microplastic treatment.

[Abstract:0054] [SERS/TERS/Plasmonics]

Polarization-Independent Dielectric Metasurfaces for Enhanced Spectroscopy

***Jose Francisco Algorri*[1], *María Gabriela Fernández-Manteca*[2], *Dimitrios Zografopoulos*[3], *Luis Rodriguez-Cobo*[1], *Adolfo Cobo*[1], *Mohammed Janneh*[4], *Patrizio Vaiano*[4], *Marco Pisco*[4], *Andrea Cusano*[4]**

[1]*Photonics Engineering Group, Universidad de Cantabria, 39005 Santander, Spain*
[2]*Instituto de Investigación Sanitaria Valdecilla, 39011 Santander, Spain*
[3]*School of Electrical and Computer Engineering, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece*
[4]*Department of Engineering, University of Sannio, Benevento, 82100, Italy*

All-dielectric metasurfaces have emerged as a highly versatile platform for engineering light-matter interactions at the nanoscale, offering a low-loss alternative to plasmonic devices for Surface-Enhanced Raman Scattering (SERS) applications. Historically, achieving the extreme electromagnetic field enhancement in these structures relies on exciting quasi-Bound States in the Continuum (qBICs) via structural symmetry-breaking. However, experimental implementations frequently reveal that quality (Q) factors are severely degraded by resonance damping caused by nanoscale fabrication vulnerabilities, such as etching roughness and statistical variations.

To overcome these vulnerabilities, we present a framework for engineering robust, high-Q resonances within fully symmetric unit cells, removing the reliance on structural asymmetry. Through Finite Element Method (FEM) and the Cartesian Multipole Decomposition Technique (CMDT) analyses, we systematically compare localized multipolar interference and delocalized Surface Lattice Resonances (SLRs) for SERS optimization.

We demonstrate that the geometric tuning of symmetric, hollow silicon nanocuboids induces the exact cancellation of Cartesian electric and toroidal dipoles, generating an ultra-high-Q state. Crucially for SERS, this architecture allows for a unique double-resonance condition. By engineering the array, we align a sharp ultra-high-Q Fano resonance (successfully tuned to the 1064 nm excitation line) alongside a broader localized Mie resonance. This overlap leverages both the intense, highly confined near-field enhancement of the sharp mode and the broader band of the localized Mie mode, making it an exceptionally powerful platform for SERS. Furthermore, this extreme localization provides remarkable immunity to environmental impedance mismatch without requiring symmetric index-matching.

Keywords: Surface-Enhanced Raman Scattering (SERS), All-dielectric metasurfaces, Surface lattice resonances, Mie resonances

[Abstract:0058] [SERS/TERS/Plasmonics]

Saliva-Based Surface-Enhanced Raman Spectroscopy For Noninvasive Detection, Typing And Localization Of Salivary Gland Tumors

***Ida Dominika Wiśniewska*[1], *Aneta Kowalska*[1], *Marta Czaplicka*[1], *Sylwia Berus*[1], *Zuzanna Gronkiewicz*[2], *Magdalena Data*[2], *Wojciech Kukwa*[2], *Agnieszka Kamińska*[1]**

[1]*Institute of Physical Chemistry Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland*
[2]*Czerniakowski Hospital, Medical University of Warsaw, ˙ Zwirki i Wigury 61, 02-091 Warsaw, Poland*

Salivary gland tumors constitute a diagnostically challenging and highly heterogeneous group of neoplasms comprising numerous benign and malignant histological subtypes. Nearly 85% arise in the parotid gland, with pleomorphic adenoma, Warthin tumor and basal cell adenoma representing the most prevalent benign entities. Their morphological complexity and overlapping cytological features frequently hinder accurate preoperative detection and typing, often necessitating imaging and invasive procedures such as biopsy for definitive characterization and anatomical localization. The development of rapid, reliable and noninvasive strategies capable of simultaneously addressing detection, differentiation and precise localization therefore remains an unmet clinical need.

Here, we propose saliva-based surface-enhanced Raman spectroscopy (SERS) as a comprehensive diagnostic platform for salivary gland tumors. Bilateral saliva samples were collected from patients with pleomorphic adenoma, Warthin tumor or basal cell adenoma and from healthy controls. Integration of SERS spectral profiling with multivariate chemometric modeling enabled robust discrimination between tumor and control groups and revealed distinct molecular fingerprints characteristic of each benign tumor type, supporting accurate tumor typing.

Crucially, comparative bilateral analysis demonstrated reproducible biochemical asymmetry between saliva secreted by the tumor-affected gland and the contralateral healthy side. This side-specific spectral divergence enabled precise localization of the diseased gland, indicating that tumor-associated molecular alterations remain spatially confined and detectable in saliva.

Collectively, these findings establish bilateral saliva-based SERS profiling combined with multivariate analysis as a rapid, label-free and noninvasive strategy integrating tumor detection, histological differentiation and gland-specific localization within a single analytical framework. This approach offers a clinically translatable alternative to invasive diagnostic procedures and may enhance preoperative evaluation and postoperative monitoring of salivary gland tumors.

Acknowledgements: This work was supported by the National Science Centre Poland OPUS 28 no 2024/55/B/ST4/01457.

Keywords: Surface-enhanced Raman spectroscopy, Salivary glands, Liquid biopsy, Tumor location, Multivariate analysis

[Abstract:0059] [Materials]

Micro-Raman Spectroscopy as a Probe of Magnetic Phase Segregation in Thermally Treated Cr_2O_3-Coated Steel

***Giulia Spaggiari*[1], *Davide Delmonte*[2], *Davide Calestani*[2], *Silvia Dante*[1], *Moia Fabio*[1], *Michele Ferri*[1], *Rosaria Brescia*[1], *Mirko Prato*[1], *Liberato Manna*[1]**

[1]*Istituto Italiano di Tecnologia (IIT), Genova, Italy*
[2]*Istituto dei Materiali per l'Elettronica e il Magnetismo, Consiglio Nazionale delle Ricerche (IMEM-CNR), Parma, Italy*

We present a correlative micro-Raman spectroscopy and SQUID magnetometry study on uncoated and Cr_2O_3-coated steel substrates, aiming to elucidate the relationship between thermally induced structural transformations and the emergence of magnetic phases. Raman spectroscopy, with its sensitivity to lattice vibrations and magnetic excitations, offers a unique window into the local chemical and magnetic ordering of these technically relevant materials.

Steel substrates were coated with a thin Cr_2O_3 layer via reactive magnetron sputtering and subsequently heat-treated at 873 K in air to simulate operational oxidation conditions. Micro-Raman spectra acquired on steel before and after treatment reveal significant modifications. In uncoated steel, thermal treatment induces the growth of characteristic iron oxide bands, indicating extensive surface oxidation. In Cr_2O_3-coated samples, the as-deposited spectra are dominated by the characteristic Cr_2O_3 phonon modes near 550 cm^{-1}. However, after air annealing, new spectral features emerge.

Crucially, the heat-treated Cr_2O_3-coated samples exhibit an additional Raman feature, which we attribute to magnon scattering. The appearance of this one-magnon mode signals the development of long-range magnetic order within the segregated oxide phases. To directly correlate these spectroscopic fingerprints with macroscopic magnetism, we performed SQUID thermal and field magnetometry on identical samples. The heat-treated chromium oxide coating significantly modifies the magnetic response of the steel substrates. A broad antiferromagnetic transition is observed around 310 K, consistent with the expected behavior of Cr_2O_3. In addition, an enhanced weak ferromagnetic remanence appears at 5 K. The coating also mitigates steel degradation, thereby suppressing the formation of iron-based secondary phases. These magnetic observations are fully consistent with the Raman spectroscopy results.

By comparing the Raman signatures with the SQUID data, we establish a correlation between specific spectral markers and the sample's magnetic properties. This preliminary work demonstrates that micro-Raman spectroscopy can serve not only as a structural probe but also as a sensitive indicator of magnetic phase segregation in coated steel systems, offering a pathway for non-destructive assessment of magnetic behavior in thermally engineered materials.

Keywords: mirco raman, magnetism, SQUID, coating, Thin films oxides

[Abstract:0062] [SERS/TERS/Plasmonics]

Comparative Evaluation of SERS Substrates for Reliable G-Quadruplex Detection

***Petra Petrović Popović*[1], *Tea Juračić*[1], *Nikša Krstulović*[2], *Snezana Miljanic*[1]**

[1]*Department of Chemistry, University of Zagreb Faculty of Science, Zagreb, Croatia*
[2]*Center for Advanced Laser Techniques, Institute of Physics, Zagreb, Croatia*

Surface-Enhanced Raman Scattering (SERS) spectroscopy is a powerful analytical tool for structural characterization of biomolecules. The quality, reproducibility, and interpretability of SERS spectra are strongly affected by the properties of the SERS substrates used in the experiment. This study presents a comparative evaluation of eight SERS substrates with respect to their performance in detecting conformational signatures of DNA G-quadruplexes.

Six colloidal suspensions of nanoparticles were synthesized by chemical reduction in solution, and two substrates were prepared by pulsed laser ablation in liquids. All substrates were comprehensively characterized by pH measurements, UV/Vis/NIR spectroscopy, scanning electron microscopy (SEM), dynamic light scattering (DLS), and zeta potential measurements. These parameters were used to establish differences in nanoparticle size, morphology, surface charge, aggregation behavior, and surface chemistry, providing a comprehensive basis for correlating substrate properties with SERS performance.

The human telomeric sequence Tel24 was used as a model system. SERS spectra were recorded for both its unfolded form and the antiparallel G-quadruplex conformation induced by high sodium ion concentrations. Comparative analysis focused on relative intensity ratios of characteristic adenine and guanine vibrational bands, which serve as structural markers for G-quadruplex folding.

Substrate performance was assessed based on the clear and reproducible detection of structure-sensitive adenine and guanine vibrational bands associated with Tel24 folding. The analysis included evaluation of relative intensity ratios of these marker bands, overall spectral clarity, background contribution, and consistency of spectral features. Differences among substrates were examined with respect to their suitability for reliable structural interpretation of unfolded and G-quadruplex conformations.

Based on the performed evaluation, citrate-stabilized silver nanoparticle colloids provided the most consistent and interpretable SERS spectra of Tel24. This work emphasized the importance of substrate selection and comprehensive physicochemical characterization for generating meaningful and reproducible SERS data in biomolecular studies. This comparative analysis provides practical insights for researchers applying SERS spectroscopy to complex nucleic acid systems.

Keywords: SERS, G-Quadruplex, Nanoparticles, Tel24, Raman Spectroscopy

[Abstract:0069] [Materials]

Analysis of Composition-Independent Local Strain in SiGe/Si Superlattices Using Raman Spectroscopy

Hyuksang Kwon

Korea Research Institute of Standards and Science

The expansion of AI-driven computing has significantly increased the demand for High Bandwidth Memory. Consequently, maintaining precise control over Ge concentration and lattice strain in SiGe/Si super-lattices has become essential for high-density integration. Although Spectroscopic Ellipsometry (SE) is widely used for non-destructive inspection of thickness and composition, it is limited in its ability to detect micro-stresses and localized strain within nanometer-sized semiconductor structures.

This study evaluates the effectiveness of Raman spectroscopy as a sensitive method for probing local strain in SiGe/Si thin films. To establish a reliable analytical framework, we used Rutherford Backscattering Spectrometry (RBS) for absolute compositional quantification of Ge content in SixGe1-x thin film. Next, High-Resolution X-ray Diffraction (HR-XRD) applied to determine in-plane and out-of-plane strain components. Comparative strain analysis revealed that Raman shifts in the Si-Si shoulder Raman band (500–518 cm^{-1}) reflect local stress variations that occur independently of changes in Ge concentration. These findings demonstrate that Raman spectroscopy, leveraging its high spatial resolution of approximately 300 nm, can analyze local strain variations and capture process-induced variables often overlooked by conventional modeling or SE-based inspection. By enabling site-specific characterization within sub-micron features, this approach offers a necessary metrology solution to complement SE, providing the physical data required for precise process control in next-generation SiGe semiconductor manufacturing.

Keywords: Raman spectroscopy, Local strain analysis, SiGe/Si super lattices

[Abstract:0081] [Coherent Raman Imaging]

Lipid Unsaturation During Dendritic Cell Maturation Revealed by Multiplex CARS Microscopy

***Kirin Yasuzaki*, Ryo Suzuki, Hideaki Kano**

Faculty of Science and Technology, Keio University, Yokohama, Japan

Dendritic cells (DCs) play a central role in the sensitization phase of type I allergy. However, the molecular mechanisms governing the transition from immature dendritic cells (iDCs) to mature dendritic cells (mDCs) remain incompletely understood. Recent studies suggests that lipid metabolism is closely linked to immune function [*Int. J. Med. Sci.* 2025, 22, 2, 417–431]. In this study, we investigated lipid compositional changes during DC maturation and explored spectroscopic markers associated with allergic sensitization.

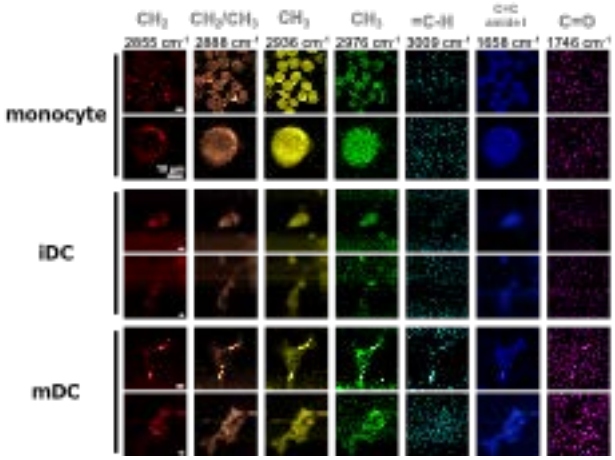
Human monocytic leukemia THP-1 cells were differentiated into iDCs, and maturarion was induced by stimulation with the model allergen ovalbumin. Label-free single-cell imaging was performed using multiplex coherent anti-Stokes Raman scattering (CARS) microscopy [*Anal. Chem.* 2025, 97, 28, 15299-15309]. The degree of unsaturation was quantified by ratio metric imaging of the Raman band at 3009 cm^{-1} (C=C stretching) relative to 2855 cm^{-1} (CH_2 stretching). Statistical significance was defined as $p < 0.05$.

CARS imaging clearly visualized intracellular lipid distributions in monocytes, iDCs, and mDCs (Fig. 1). Compared with iDCs, mDCs exhibited pronounced accumulation of cytoplasmic lipid droplets. Quantitative ratio imaging and histogram analysis of the 3009/2855 cm^{-1} signal demonstrated a significant increase in lipid unsaturation in mDCs relative to iDCs ($p < 0.05$, Fig.2). These results indicate that DC maturation involves not only increased lipid accumulation but also compositional remodeling toward higher unsaturation.

In conclusion, we demonstrate that lipid unsaturation increases during DC maturation. The 3009/2855 cm^{-1} ratio serves as a quantitative spectroscopic marker of DC activation and provides new insight into the metabolic regulation associated with allergic sensitization.

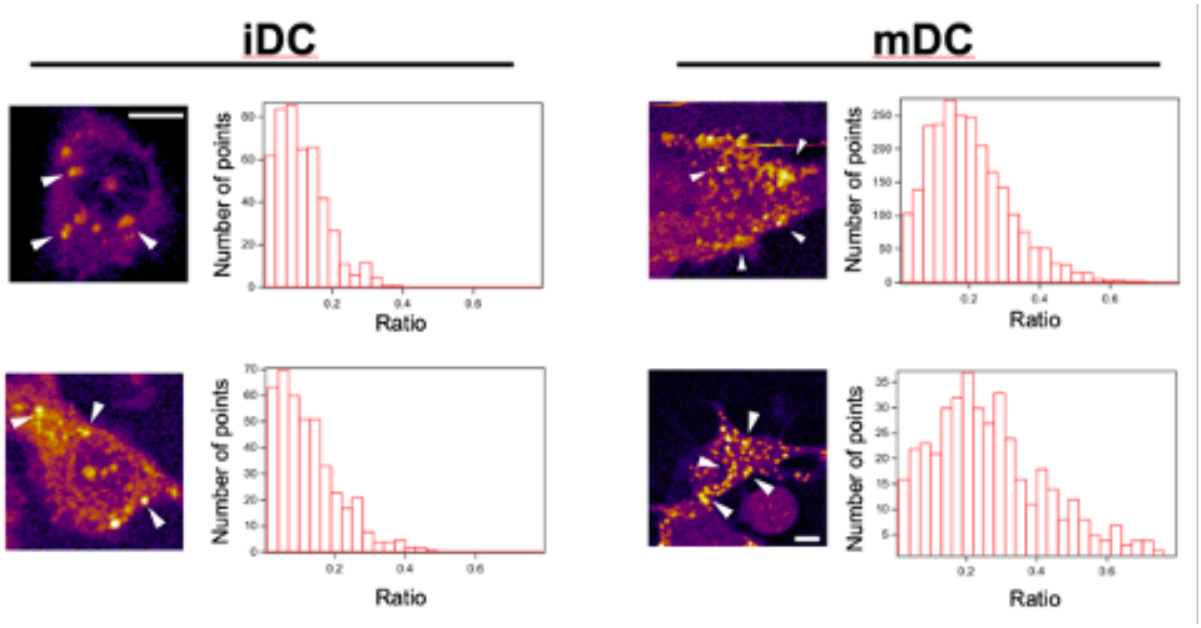
Keywords: CARS, Microscopy, Live cell

1



CARS images of monocytes, iDCs, and mDCs. Two representative images for each condition are shown.Scale bar: 10 μm.

2



Quantitative analysis of lipid unsaturation in iDCs and mDCs. Representative images are shown.

[Abstract:0089] [SERS/TERS/Plasmonics]

Bacterial Detection in Wound Infections Using Highly Porous, Flexible and Biocompatible SERS Substrates

***David Miguel Henriques Bento*[1], *Gohar Soufi*[1], *Fatemeh Ajalloueian*[1], *Lars Jelsbak*[2], *Anja Boisen*[1]**

[1]*Department of Health Technology, Technical University of Denmark, Kgs. Lyngby, Denmark*
[2]*Department of Biotechnology and Biomedicine, Technical University of Denmark, Kgs. Lyngby, Denmark*

Chronic wound infections in hospitalized patients remain a significant medical challenge, leading to prolonged hospital stays, high mortality rates, and substantial healthcare costs [*Advances in Wound Care*. 2021;10(5):281-292]. When a wound infection is suspected, samples are sent to a laboratory for bacterial identification using colony culture methods, which typically takes several days. During this time, infections can worsen or spread, potentially leading to systemic complications. This is especially problematic with antibiotic resistant and opportunistic bacteria such as *Pseudomonas aeruginosa* and *Staphylococcus aureus*.

This study uses high porosity substrates of electrospun polyamide 11 patches for efficiently sampling and identifying bacterial biomarkers from wound exudates. Star shaped gold nanoparticles were grown on the fibers' surface to make them SERS active, enabling rapid infection biomarker detection. The patches' biocompatibility and flexibility ensure adaptability to uneven wound surfaces. Coupled with automated machine learning, such as SIMCA, PLS-DA, this system streamlines diagnostics, minimizing sample preparation and turnaround times (Figure 1). It facilitates early infection detection, guiding antimicrobial therapy, and reducing the healthcare burden of wound infections.

Keywords: SERS, Diagnostic, Metabolites, Nanoparticles, Biocompatible, Flexible

Graphical abstract

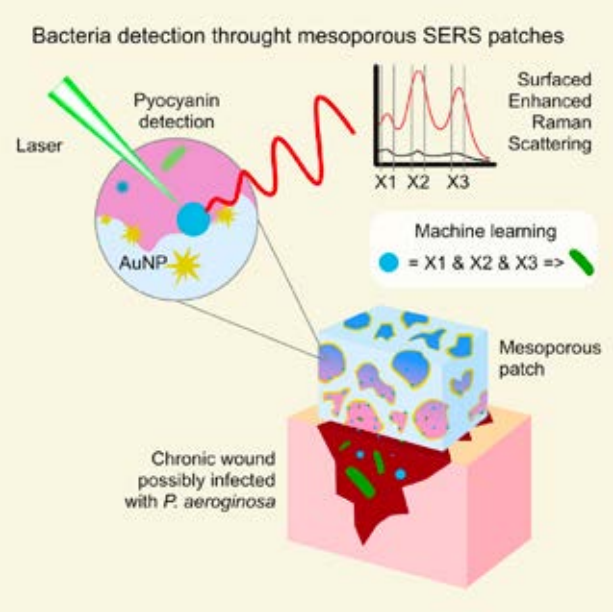


Figure 1 - Sampling of bacterial metabolites and detection of bacteria via classification using metabolites' SERS

[Abstract:0095] [Planetary/Geosciences]

Advancing Geochemical Characterisation Through Confocal and 3D Raman Microscopy

Iona Elizabeth Hill

Edinburgh Instruments, Livingston, UK

Raman spectroscopy is increasingly recognised as a versatile and non destructive tool for geochemical investigation, offering rapid access to molecular and structural information across a wide range of geological materials. In this work, we demonstrate the breadth of capability provided by modern confocal and three dimensional Raman microscopy for applications spanning mineral identification, phase discrimination, and the analysis of micro scale heterogeneity within geological samples.

The use of integrated spectral databases supports confident material assignment in both simple and compositionally complex systems, while Raman mapping approaches - including surface mapping methods - enable chemical imaging of samples that exhibit natural topographic variation. Additionally, 3D Raman imaging provides enhanced insight into the spatial arrangement and composition of inclusions and other fine scale features, allowing characterisation without the need for destructive sample preparation.

Overall, this work highlights the flexibility of Raman microscopy as a tool for geochemical characterisation. Its ability to interrogate diverse, heterogeneous geological materials with minimal preparation underscores its value for both routine and advanced analytical workflows in modern geoscience.

Keywords: Raman Spectroscopy, Geochemistry, Geochemical Characterisation

Posters

[Abstract:0097] [Novel Approaches]

VibSpecDB: a FAIR-Oriented İnfrastructure For Raman and IR Spectroscopy Data

Darina Stefaniuk*, *Thomas Bocklitz

Leibniz Institute of Photonic Technology, Albert Einstein Strasse 9, 07745 Jena, Friedrich Schiller University Jena, Institute of Physical Chemistry (IPC) and Abbe Center of Photonics (ACP), Helmholtzweg 4, 07743 Jena, Germany

Vibrational spectroscopy methods, including Raman and infrared (IR) spectroscopy, are increasingly applied across materials science, chemistry, and life sciences. However, despite the continuous growth in the volume and diversity of generated data, specialized FAIR-oriented infrastructures for the structured management of vibrational spectroscopy data remain scarce. Many existing solutions are either reference-focused or fragmented, and they rarely support the full workflow from data acquisition to analysis and reuse. VibSpecDB has been developed to address this gap.

VibSpecDB is implemented as a web-based application using modern technologies to ensure secure storage of both personal and scientific data. The system provides structured data organization, annotation, and search functionality, enabling stored datasets to be directly used in downstream analysis workflows. VibSpecDB follows a hierarchical data model (Project–Study–Dataset), allowing metadata and tags to be assigned at all levels of data organization. Metadata can be provided either through structured CSV files or via flexible inputs of key–value pairs within the graphical user interface.

The repository supports search and filtering across Projects and Studies based on metadata or tags, as well as data export and in-platform visualization of spectral data. VibSpecDB is implemented as a containerized system and deployed within a cloud-based Kubernetes infrastructure, supporting modular development and scalability.

The system is currently available as a live deployment and is under active development. Ongoing work focuses on implementing a structured publication and validation workflow, dataset versioning, alignment with standardized metadata schemas, and harmonization with federation services within NFDI4Chem.

Acknowledgement: Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – 441958208. This work is additionally supported by the BMBF, funding program Photonics Research Germany (13N15708 (LPI-BT3)) and is integrated into the Leibniz Center for Photonics in Infection Research (LPI). The LPI initiated by Leibniz-IPHT, Leibniz-HKI, Friedrich Schiller University Jena and Jena University Hospital is part of the BMBF national roadmap for research infrastructures.

Keywords: repository, infrastructure,metadata

Posters

[Abstract:0098] [Biology/Biomedicine]

Raman Profiling Reveals LRG1-Dependent Shifts in CAF-Linked Biochemical Features in PDAC

***Ye Lin Yang*[1], *Eunsung Lee*[2], *Si Yeon Han*[3], *Heesuk Rho*[2], *Jimin Yang*[3]**

[1]*JBNU G-LAMP Project Group, Research Institute for Materials and Energy Sciences (RIMES), Jeonbuk National University, Jeonju 54896, Republic of Korea*
[2]*Department of Physics, Jeonbuk National University, Jeonju, 54896, Republic of Korea*
[3]*Department of Molecular Biology, Jeonbuk National University, Jeonju, 54896, Republic of Korea*

Pancreatic ductal adenocarcinoma (PDAC) remains a highly lethal malignancy, in large part because dense fibrosis limits the benefit of surgery and conventional chemotherapy. Cancer-associated fibroblasts (CAFs) are central organizers of the tumor microenvironment (TME), shaping tumor growth, immune contexture, and therapy resistance. Leucine-rich alpha-2-glycoprotein 1 (LRG1) has been reported as a prognostic biomarker in plasma and tumor tissue from pancreatic cancer patients, and its expression is closely associated with CAF-rich stroma. However, whether LRG1 actively modulates CAF-associated phenotypes and stromal architecture in PDAC remains poorly defined.

To interrogate LRG1 function in vivo, we compared tumor burden and survival between wild-type (WT) and LRG1 knockout (KO) mice using an orthotopic pancreatic cancer model followed for 21 days. LRG1 KO mice showed improved survival and significantly smaller tumors relative to WT controls. Stromal collagen organization was evaluated by second-harmonic generation (SHG) imaging and immunohistochemistry (IHC). For label-free biochemical phenotyping, Raman spectroscopic mapping was performed on consecutive tissue sections aligned with IHC.

Raman analysis suggested LRG1-associated spectral patterns within the stromal compartment. Relative to WT tumors, LRG1 KO tumors tended to show higher signals in bands linked to myCAF-associated components, including the guanine band at 680 cm^{-1} and collagen-related peaks across 481–1175 cm^{-1}. Lipid-associated peaks at 2896, 2910, and 2950 cm^{-1} would be examined as potential features related to iCAF-like states, given expected inter-sample variability. Taken together with SHG and IHC, these observations are consistent with the possibility that LRG1 is associated with shifts in CAF-related stromal features and fibrotic remodeling in PDAC.

Overall, Raman spectroscopy integrated with IHC-guided spatial validation provides a practical platform for quantifying LRG1-linked stromal phenotypes in situ and defining spectral biomarkers that may inform stromal-targeted intervention strategies.

This study was supported by the National Research Foundation of Korea (NRF) grants funded by the Korean government (MSIT) (No. RS-2025-16067187), and the G-LAMP Program of the NRF grant funded by the Ministry of Education (No. RS-2024-00443714).

Keywords: LRG1, pancreatic ductal adenocarcinoma, tumor microenvironment, Raman spectroscopy

[Abstract:0100] [Materials]

Spatially Resolved Raman Spectroscopy of Janus Monolayers

***Eunsung Lee*[1], *Taegeon Lee*[1], *Swathi Krishna*[2], *Ki Kang Kim*[2], *Heesuk Rho*[1]**

[1]*Department of Physics, Research Institute for Materials and Energy Sciences, Jeonbuk National University, Jeonju, Republic of Korea*
[2]*Department of Energy Science, Sungkyunkwan University, Suwon, Republic of Korea*

Janus transition metal dichalcogenides exhibit distinct optical anisotropy arising from broken out-of-plane inversion symmetry. Here, we report Raman spectroscopic mapping of Janus WSSe monolayers. The Janus WSSe was fabricated from monolayer WS2 grown on a gold substrate via chemical vapor deposition. The top-layer sulfur atoms were selectively removed using hydrogen plasma–assisted etching, enabling their subsequent replacement with selenium atoms. Raman spectra reveal characteristic phonon peaks at approximately 283 cm^{-1} and 339 cm^{-1}, corresponding to the out-of-plane and in-plane vibrational modes, respectively. These Raman features exhibit significant variations with excitation wavelength, primarily due to resonance effects associated with the electronic band structure. Detailed phonon analysis provides spectroscopic evidence that the monolayer forms an atomically ordered Janus structure rather than a random alloy. Raman mapping performed over the entire surface of individual WSSe monolayers reveals distinct differences in phonon characteristics between the central and edge regions of large monolayer flakes, including variations in wavenumber, linewidth, and intensity, whereas such variations are absent in relatively small flakes. These results indicate that spatial structural variations occur only in large flakes. Despite these morphological differences, the polarized Raman responses obey the expected Raman polarization selection rules regardless of flake size, indicating the high crystalline quality of the Janus monolayers. Consequently, this spectroscopic approach provides a robust metric for evaluating the quality of emerging two-dimensional functional materials and offers insights for future photonic and optoelectronic device applications.

[This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (Grant No. RS-2025-23324133) and the G-LAMP Program of the NRF grant funded by the Ministry of Education (Grant No. RS-2024-00443714).]

Keywords: Janus monolayer, Raman spectroscopy, Optical phonon

[Abstract:0108] [Industrial/Societal Applications]

Interlaboratory Comparison for Determining the Number of Graphene Layers and Characterizing Graphene Powders Using Raman Microscopy

***Alessio Sacco*[1], *Mark A. Bissett*[3], *Ian A. Kinloch*[3], *Alexandra Delvallée*[4], *Sébastien Ducourtieux*[4], *Kiran Subhedar*[5], *All Participants To The Comparison*[6], *Keith R. Paton*[2], *Andrew J. Pollard*[2], *Charles A. Clifford*[2], *Chiara Portesi*[1], *Andrea M. Rossi*[1]**

[1]*Istituto Nazionale di Ricerca Metrologica (INRiM), Torino, Italy*
[2]*National Physics Laboratory (NPL), Teddington, United Kingdom*
[3]*University of Manchester, Manchester, United Kingdom*
[4]*Laboratoire National de Métrologie et d'Essais (LNE), Trappes, France*
[5]*National Physical Laboratory (CSIR-NPLI), New Delhi, India*
[6]*Various institutions and industries worldwide*

Graphene, as the first synthetized type of the expanding family of truly two-dimensional materials, hold great promise for many high-impact applications, including flexible electronics, energy storage, and biosensors. Despite a growing number of global producers has appeared in the last years, the industry is hampered by the lack of definitions and quality control standards: materials are often poorly characterized, exhibit high batch-to-batch variation, and are frequently mislabeled, with few distinguishing between actual graphene and other two-dimensional graphene-related materials (GR2M). This inconsistency, where products described as graphene are often closer to graphite, undermines the commercialization and application of these materials. A critical obstacle to establishing reliable standards is the need for proven, verifiable characterization methods applicable to cost-effective, scalable products such as GR2M powders, which must be validated through rigorous interlaboratory studies.

More than 12 laboratories participated in the international interlaboratory comparison (ILC) here presented, conducted in the Versailles Project on Advanced Materials and Standards (VAMAS) framework. It focused on the validation of operating procedures aimed at graphene nano-platelets characterization by Raman spectroscopy, leveraging its advantages as a fast, widespread, and non-destructive analytical tool. The effort was twofold: commercially available graphene powders were used for the development of nano-platelets localization and Raman mapping protocols with a specifically developed substrate; furthermore, high-quality mechanically exfoliated graphene was used for the assessment of a simplified method for the quantification by Raman of the number of layers, verified by atomic force microscopy. These procedures for the measurement and interpretation of graphene Raman spectra, developed to be simple and unambiguous, are thus suitable candidates for being disseminated and adopted as standards. The results of this ILC will be used as input into ISO TC229 JWG2 for the upcoming revision of ISO/TS 21356-1 "Structural Characterization of Graphene". The results will benefit the entire graphene supply chain, both manufacturers and end-users, by establishing globally characterization procedures towards accepted material specifications. Raman spectroscopy offers a unique fingerprint for graphene, providing a critical method for agile layer number measurement.

Keywords: Graphene, Graphene Powders, Interlaboratory Comparison, Standardization, Metrology, GR2M (graphene-related 2D materials)

[Abstract:0116] [SERS/TERS/Plasmonics]

Electrochemically-Etched Micro-Macroporous Silicon for SERS Analysis of Complex Samples

***Doohong Min*, Taeyeong Kim, Jungchul Lee**

Korea Advanced Institute of Science and Technology

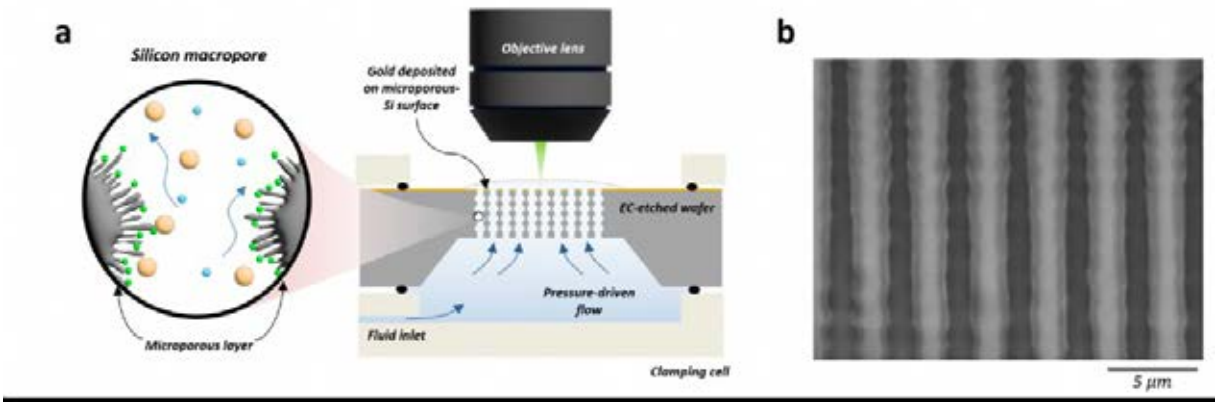
Surface-enhanced Raman spectroscopy (SERS) enables ultrasensitive molecular detection, but direct analysis of complex samples is often limited by matrix interference. Here, we propose a monolithic silicon-based micro total analysis system (MicroTAS) that integrates continuous in-flow sample pretreatment with top-surface SERS detection. As illustrated in Fig. a, the platform guides the sample from a bottom flow cell through a through-silicon porous architecture to a SERS-active top surface.

The device consists of a high-aspect-ratio silicon macropore via array fabricated by electrochemical etching, with pore diameters of 1–3 μm and lengths exceeding 50 μm. Periodically modulated via diameters were also realized to tailor pore geometry. Backside KOH etching was then used to open the pores completely, forming through-silicon vias that allow upward pressure-driven flow. During transport, the functionalized internal via surface enables in situ sample capture and cleanup. As shown in Fig. b, cross-sectional SEM imaging confirms the fabricated macropore array and the microporous layer formed along the pore walls.

The pretreated analytes subsequently reach the top-surface microporous layer coated with a thin gold nanofilm, where dense plasmonic hot spots enhance the Raman signal while suppressing the photoluminescence background of porous silicon. This integrated architecture provides a practical route for combining sample transport, pretreatment, and sensitive optical detection within a single silicon chip.

Keywords: Electrochemical etching, Silicon macropore array, SERS

Figure 1.



(a) Schematic of a micro-TAS flow cell based on electrochemically etched silicon macro-/microporous structures. (b) Cross-sectional SEM image of electrochemically etched silicon macroporous structures.

[Abstract:0119] [SERS/TERS/Plasmonics]

Probing Biomolecules Using Surface Enhanced Linear and Nonlinear Raman Scattering

***Fariha Binte Rahman*[1], *Maria Eleonora Temperini*[2], *Alexander Veber*[2], *Janina Kneipp*[1]**

[1]*Department of Chemistry, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 2, 12489 Berlin, Germany*
[2]*Institute for Electronic Structure Dynamics (PS-IESD), HZB-BESSY, Albert-Einstein-Str. 15, 12489 Berlin, Germany*

Plasmonic nanostructures provide highly localized electromagnetic enhancement that can be harnessed, e.g., for ultrasensitive spectroscopy applications. However, the molecular orientation and structure of the analyte molecules at the surface of the nanostructures and in their high local fields are also impacted. Surface enhanced Raman scattering (SERS) and its two-photon analogue surface enhanced hyper Raman scattering (SEHRS) give us insights into changes that are specific to metal-molecule interactions. Specially SEHRS has shown more sensitivity towards minuscule changes in local environments. Nevertheless, finding a plasmonic metal substrate suitable for SEHRS is challenging because of the large gap between excitation and detection wavelengths and the strong influence of chemical enhancement in the process.

In this work, we discuss surface enhanced vibrational spectra of biomolecules, ranging from aromatic amino acids to whole proteins, under non-resonant conditions, obtained with spherical gold nanoparticles of different sizes as plasmonic substrate. We show that the spectral differences in the relative signal intensities and particular vibrational modes are due to different selection rules, as well as from the functional groups specific to the different molecules. The data demonstrate good agreement with previous work that used silver nanostructures. The spectra also indicate high sensitivity to specific molecule-nanostructure interactions. The information from SERS and SEHRS was combined with the nano-infrared spectra collected from similar samples using a scattering type scanning near field microscope. We demonstrate that combining the different techniques affords a comprehensive understanding of formation of protein-nanoparticle agglomerates under different experimental conditions. With this multimodal spectroscopic approach, we expect to study more complex systems in the future.

Keywords: Surface enhanced Raman scattering (SERS), Surface enhanced hyper Raman scattering (SEHRS), biomolecules, gold nanoparticles

Posters

[Abstract:0132] [SERS/TERS/Plasmonics]

Hotspot-Rich, TLC-Integrated Ni@Au/Ag Trimetallic SERS Substrates for On-Site Trace Detection of Explosives, Drugs, and Pesticides

Shashikana Paria[1], ***Prasenjit Maity***[2]

[1]*School of Engineering and Technology, National Forensic Sciences University, Gandhinagar -382007, India*
[2]*School of Engineering and Technology, National Forensic Sciences University, Guwahati -781032, India*

Rapid, on-site identification of trace explosives, drugs, and pesticide residues remains a persistent need in security screening, forensic investigations, and environmental monitoring. Here we report a robust trimetallic SERS platform based on Ni@Au core–shell nanoparticles decorated on plasmonic Ag nanoplates (Ni@Au/Ag) and integrated onto a low-cost, mechanically stable TLC-plate support to create a ready-to-use sensing substrate. The design combines (i) high-density electromagnetic hot spots arising from nano-gaps and nano-cavities between Ni@Au nanoparticles and Ag nanoplates, and (ii) chemical enhancement enabled by interfacial charge redistribution and charge-transfer pathways across Ni/Ag–Au interfaces.

Using a single 785 nm excitation, the substrate provides label-free, non-destructive, and multiplex Raman fingerprinting across chemically diverse targets, including major explosives (e.g., RDX, PETN, DNT/TNT/TNP-class analytes), representative drugs (e.g., naproxen, paroxetine), and pesticides (e.g., carbofuran, malathion, chlorpyrifos). Concentration-dependent SERS signatures are obtained from solution-drop deposition, with detectable fingerprints down to the low-micromolar range (down to ~1 μM for key explosives such as RDX and PETN) under the reported measurement conditions. Finite-element electromagnetic simulations (COMSOL, Wave Optics with PML boundaries) support the experimentally observed enhancement trends and provide structure–performance insight into field localization within the hybrid architecture. Practical relevance is demonstrated via a spiking–recovery test on fabric, where ethanol extracts from apron surfaces spiked with RDX and TNP yield clear diagnostic Raman bands on the developed substrate.

Overall, this Ni@Au/Ag-on-TLC format offers a scalable route to sensitive, portable SERS screening for real-world forensic and environmental samples.

Keywords: SERS, trimetallic nanostructures, explosives detection, pesticide sensing, hot spots

[Abstract:0137] [Materials]

Resonance Raman Study of Differing Electronic Transitions in Acceptor-Donor-Acceptor Compounds

***Sana Maroof*, Keith Gordon**

Department of Chemistry & MacDiarmid Institute, University of Otago, Dunedin, NEW ZEALAND

In this study, we investigate a series of Acceptor–Donor–Acceptor (A–D–A) compounds designed with differing core units and peripheral acceptor groups. The structural modification of the central donor core contains either benzothiadiazole (BTD) or benzodithiophene (BDT). For the acceptor units these include indandione, malononitrile and dimalononitrile. Both types of units tune the properties with the optical bandgap being tuned between λmax = 512 to 639 nm. Emission spectra showed some interesting solvatochromic properties. The BDT core compounds show distinct shifts in the emission spectra with solvent - those with BTD do not. This points to differing types of transitions and these are explored using resonance Raman spectroscopy.

Density Functional Theory (DFT) calculations validated the experimental findings; B3LYP provided a superior description of UV–Vis electronic transitions, while CAM-B3LYP accurately reproduced vibrational fingerprints observed in FT-Raman spectra. Resonance Raman analysis, conducted across multiple excitation wavelengths, confirmed that BDT-based compounds exhibit significant enhancement of carbonyl (C=O) stretching and aromatic skeletal modes. This selective enhancement provides direct evidence of the different nature of electronic transitions between the BTD and BDT series, particularly highlighting the role of strong Internal Charge Transfer (ICT) in the latter. Furthermore, Natural Population Analysis (NPA) quantified the transition-specific charge redistribution, correlating the experimental vibrational intensity shifts with the calculated electronic excited-state dynamics.

Keywords: Resonance Raman Spectroscopy, A-D-A Molecules, Charge Transfer

[Abstract:0138] [SERS/TERS/Plasmonics]

Plasmonic Momentum Engineering of Raman Scattering at the Subnanometer Scale

***Norihiko Hayazawa*[1], *Maria Vanessa Balois Oguchi*[2], *Yuto Fujita*[3], *Tomoko Shimizu*[3], *Takuo Tanaka*[1]**

[1]*RIKEN Center for Advanced Photonics, RIKEN, Wako, Saitama, Japan*
[2]*Department of Electrical and Electronic Engineering, Institute of Science Tokyo, Yokohama, Kanagawa, Japan*
[3]*Department of Applied Physics and Physico-Informatics, Keio University, Yokohama, Kanagawa, Japan*

Since Abbe's diffraction limit was long regarded as a fundamental barrier in optical microscopy, the emergence of super-resolution techniques such as PALM and STED, recognized by the 2014 Nobel Prize in Chemistry, revolutionized fluorescence imaging. However, this breakthrough has remained largely confined to fluorescence-based approaches. In the 2009 Nature Photonics focus issue on imaging beyond the diffraction limit, Kawata and co-workers emphasized that plasmonics could extend super-resolution concepts beyond fluorescence, potentially transforming other spectroscopies [1].

Here we demonstrate that plasmonically confined near-field light does not merely improve spatial resolution in Raman spectroscopy, but fundamentally reshapes its selection rules. Using subnanometer-resolution tip-enhanced Raman spectroscopy (TERS) under ambient conditions [2], we establish a unified framework of plasmonic momentum engineering of Raman scattering.

In defect-free graphene, dipole-forbidden phonon modes (D, D′) and even combination modes (D + D′) become activated without structural defects [3,4]. In metallic carbon nanotubes, polarization-dependent resonance Raman pathways are modified, enabling non-vertical electronic transitions in k-space [5]. In strained graphene nanostructures, the near-field-induced D-band intensity scales with lattice deformation and the finite number of hexagonal units within the plasmonic cavity [6,7]. Across these systems, the breakdown of the dipole approximation arises from the large field gradients and high in-plane momentum components generated in the plasmonic nano-cavity.

These findings position subnanometer TERS not simply as an extension of surface-enhanced Raman scattering (SERS), but as a new spectroscopic regime in which plasmonic confinement engineers light–matter interaction at the fundamental level. Extending super-resolution concepts from fluorescence to vibrational and electronic transitions, plasmonic momentum engineering opens a pathway toward symmetry-controlled nanoscale spectroscopy and transition-selective optical physics.

References:

[1] "Beyond the diffraction limit", Nature Photon. 3, 361 (2009)
[2] M. V. Balois, et al., Jpn. J. Appl. Phys., 58, SI0801 (2019).
[3] K. Ikeda, et al., J. Am. Chem. Soc., 135, 11489 (2013).
[4] M. V. Balois, et al., npj 2D Mater. Appl., 3, 38 (2019).
[5] Y. Fujita, et al., J. Appl. Phys. 135, 193101 (2024).
[6] M. V. Balois-Oguchi, et al., 127, 5982 (2023).
[7] Y. Fujita, et al., Appl. Spectrosc. 80, 51 (2025).

Keywords: Plasmon, TERS, polarization, subnanometer

Posters

[Abstract:0140] [Biology/Biomedicine]

Raman Spectroscopy and AFM Reveal LRG1 Dependent Biochemical and Mechanical Remodeling During Hepatic Stellate Cell Activation

***Gahi Hong*[1], *Eunsung Lee*[2], *Hyunji Shin*[1], *Daekwon Lee*[2], *Heesuk Rho*[2], *Jimin Yang*[1]**

[1]*Department of Molecular Biology, Jeonbuk National University, Jeonju, Republic of Korea*
[2]*Department of Physics, Research Institute for Materials and Energy Sciences, Jeonbuk National University, Jeonju, Republic of Korea*

Fibrosis develops when hepatic stellate cells (HSCs) are activated after liver injury and transition to a myofibroblast-like state, driving excessive extracellular matrix (ECM) accumulation and increased α-smooth muscle actin expression. Leucine-rich α-2-glycoprotein 1 (LRG1) is a secreted protein linked to inflammation and angiogenesis, and Latrophilin-2 (LPHN2) has been proposed as a receptor for LRG1. However, it remains unclear whether LRG1 promotes HSC activation through an LPHN2-dependent mechanism. Here, we profiled early biochemical and biophysical changes during LRG1-driven HSC activation using Raman spectroscopy and atomic force microscopy (AFM).

Wild-type (WT) and LPHN2-knockout (KO) HSCs generated by CRISPR–Cas9 were treated with recombinant LRG1 and analyzed. Raman spectroscopy captured group-level spectral changes with emphasis on the Raman bands associated with cytochromes, lipids, proteins, and nucleic acids. In parallel, AFM quantified changes in elastic modulus and cell height.

In WT HSCs, LRG1 increased Raman signals originating from cytochromes, unsaturated lipids, and protein-associated bands, while signals linked to saturated lipids and nucleic acids decreased. These spectral changes matched mechanical remodeling. AFM showed a marked increase in elastic modulus, accompanied by reduced cell height, supporting a myofibroblast-like phenotype. In contrast, LPHN2-KO cells showed minimal spectral and mechanical responses to LRG1 and largely retained a quiescent profile.

Together, these results indicate that the LRG1–LPHN2 axis coordinates biochemical composition and mechanical properties during HSC activation. The combined Raman–AFM approach provides a label-free measure of early activation states that may be useful for tracking fibrotic progression.

This study was supported by the National Research Foundation of Korea (NRF) grants funded by the Korean government (MSIT) (No. RS-2025-16067187), and the G-LAMP Program of the NRF grant funded by the Ministry of Education (No. RS-2024-00443714).

Keywords: LRG1, LPHN2, fibrosis, Raman spectroscopy, atomic force microscopy (AFM)

[Abstract:0141] [Biology/Biomedicine]

Raman Spectroscopic Analysis of Microplastic–Cellular Interactions

***Jiho Park*[1], *Yeonju Park*[2], *Young Mee Jung*[2]**

[1]*Department of Chemistry, Institute for Molecular Science and Fusion Technology, Kangwon National University, Chuncheon 24341, Korea*
[2]*Department of Chemistry, Institute for Molecular Science and Fusion Technology, Kangwon National University, Chuncheon 24341, Korea, Kangwon Radiation Convergence Research Support Center, Kangwon National University, Chuncheon 24341, Korea*

Microplastics (MPs) are solid plastic particles smaller than 5 mm in diameter that are widely distributed throughout the environment.[1] They are increasingly recognized as emerging contaminants capable of inducing cellular toxicity, including oxidative stress, inflammation, and apoptosis. Once internalized by cells, MPs can disrupt the composition and structural organization of essential biomolecules such as lipids, proteins, and nucleic acids.

To date, most studies evaluating the biological effects of MPs have employed sterilized particles. To more realistically simulate environmental exposure conditions, we compared the Raman spectra of cells exposed to MPs before and after sterilization. The detailed results and their implications will be presented and discussed.

Reference:

[1] K.T. Ho, R. Bjorkland, R. M. Burgess, Comparing the definitions of microplastics based on size range: Scientific and policy implications, *Mar. Pollut. Bull.*, 207, 116907 (2024)

Keywords: Microplastics, Raman spectroscopy, Cellular toxicity

[Abstract:0144] [SERS/TERS/Plasmonics]

Study of Simple Template MIP via LSPR-Raman

***Ester Iatta*[1], *Tolga Zorlu*[2], *Jia Min Chin*[2], *Peter Lieberzeit*[3]**

[1]*Doctoral School of Chemistry (DoSChem), Department of Physical Chemistry, University of Vienna, Vienna, Austria*
[2]*Department of Functional Materials and Catalysis, University of Vienna, Vienna, Austria*
[3]*Department of Physical Chemistry, University of Vienna, Vienna, Austria*

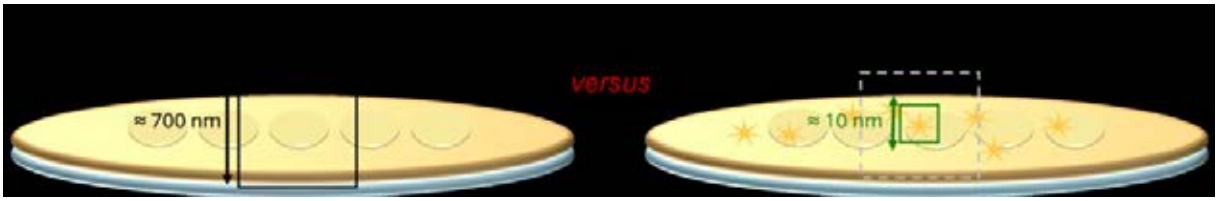
Molecularly Imprinted Polymers (MIPs) are a particular class of polymeric materials designed to be selective for detecting a specific analyte. The main concept behind them is to allow the monomers to arrange around a template thanks to affine functional groups. Once the curing step is complete, the template can be removed and rebound as analyte.

Vast literature has been produced on MIPs applications in analytical chemistry; however, direct characterization of the MIP's selective region (also known as cavity) is very challenging. Indeed, structural models of cavities mostly rely on theoretical calculations and affinity tests. Herein, we aim at developing a method to observe the cavities or selective regions directly.

Therefore, we chose to deposit gold nanostars (AuNSts) onto styrene-co-ethylene glycol dimethacrylate imprinted layers followed by Raman measurements to characterize the surface features of the described substrate. The rationale behind the approach is that localized surface plasmon resonance Raman (LSPR-Raman) concentrates the signal in the closest surroundings of the nanomaterial which leads to maximum enhancement. This will allow the Raman signal of the MIP's interface to be more intense than the signal originated from the bulk polymer. It is worth noting that this setup reverses the conditions usually experienced during Raman Spectroscopy: while standard Raman spectra show primarily characteristic signals of the polymer bulk, the most prominent bands in LSPR-Raman will be the ones originating from the material's interface (Fig.1).

Keywords: molecularly imprinted polymers, LSPR-Raman, in depth characterization, sensing

Fig. 1



Schematic representation of Molecularly Imprinted Polymer and probed volume with Raman Spectrocopy.

[Abstract:0150] [Biology/Biomedicine]

Synthetic Melanin as a Bioinspired Antioxidant: Raman Spectroscopic Validation of Redox Protection in Human Skin

***Mohamed Touhid Patel*[1], *Aditi Vichare*[2], *Sourav Mukherjee*[2], *Abhijit Majumder*[2], *Pola Goldberg Oppenheimer*[1]**

[1]*Advanced Nanomaterials Structures and Applications Laboratories, School of Chemical Engineering, College of Engineering and Physical Sciences, University of Birmingham, Edgbaston, Birmingham, B15 2TT, UK*
[2]*Department of Chemical Engineering, Indian Institute of Technology Bombay, Mumbai, 400076, India*

Oxidative stress is a major driver of epidermal dysfunction, contributing to DNA damage, impaired barrier integrity, and delayed tissue repair. Although endogenous melanin provides intrinsic antioxidant protection in skin, its therapeutic translation is limited by poor solubility and structural heterogeneity. In this study, we investigated whether commercially available synthetic melanin (SynMel) can function as an intracellular antioxidant and protect epidermal structure under chemically induced oxidative stress.

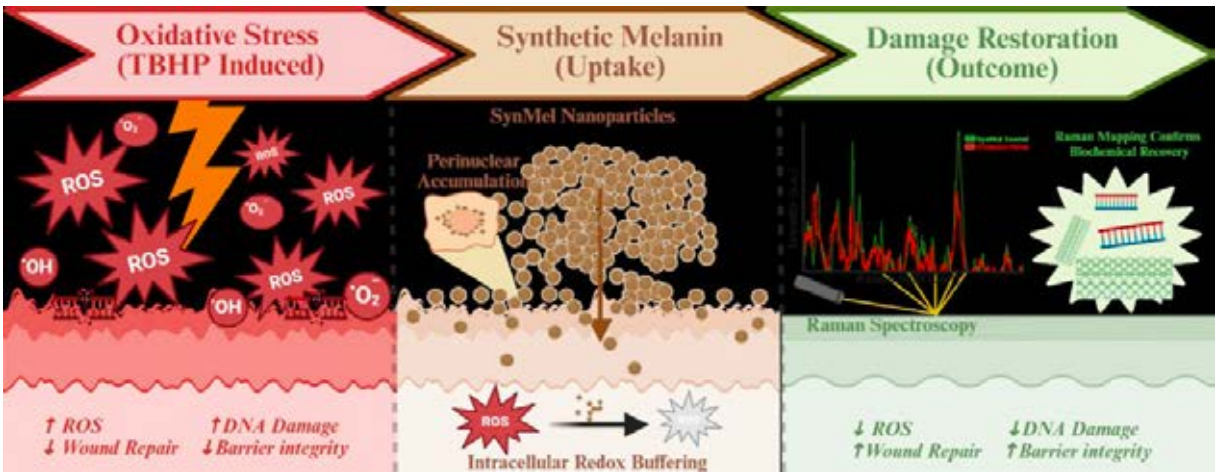
Human keratinocytes (HaCaT) were treated with SynMel (1–6 μM) prior to oxidative challenge using tert-butyl hydroperoxide (TBHP). SynMel was efficiently internalised by keratinocytes and significantly reduced intracellular reactive oxygen species (ROS) and γ-H2AX–associated DNA damage. Functional assays demonstrated improved keratinocyte migration and preservation of epithelial barrier integrity under oxidative stress conditions.

To validate these protective effects at the tissue level, label-free Raman spectroscopy was performed on ex vivo human skin explants. TBHP exposure produced marked attenuation of Raman bands associated with proteins, lipids, and aromatic amino acids, indicating oxidative biochemical damage. SynMel treatment restored key spectral features, including phenylalanine (~1003 cm^{-1}) and CH_2/CH_3 lipid bands (~1440–1470 cm^{-1}), demonstrating recovery of epidermal biochemical integrity. Multivariate analysis further confirmed clustering of SynMel-treated samples closer to untreated controls.

Together, these results demonstrate that synthetic melanin functions as a bioinspired intracellular redox modulator that mitigates oxidative damage at both cellular and tissue levels. This work highlights the utility of Raman spectroscopy as a powerful label-free tool for evaluating antioxidant mechanisms in human skin and supports the translational potential of synthetic melanin in oxidative stress–related dermatological conditions (Graphical Abstract).

Keywords: Synthetic melanin, Oxidative stress, Keratinocyte, Skin barrier function, Raman spectroscopy, Ex vivo human skin

Graphical Abstract



[Abstract:0154] [Novel Approaches]

Minimum Information About Chemical Investigation (MIChI) For Raman Assays

***Noura Rayya*[1], *Giacomo Lanza*[2], *Darina Stefaniuk*[3], *Nicole Jung*[4], *Philip Strömert*[1], *Oliver Koepler*[1], *Steffen Neumann*[5], *Thomas Bocklitz*[3]**

[1]*Lab Scientific Knowledge, TIB – Leibniz Information Centre For Science And Technology, Hanover, Germany*
[2]*Scientific Libraries, Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany*
[3]*Photonic Data Science, Leibniz Institute Of Photonic Technologies, Jena, Germany*
[4]*Institute Of Biological And Chemical Systems (IBCS), Karlsruhe Institute Of Technology (KIT), Eggenstein-Leopoldshafen, Germany*
[5]*Computer-Aided Plant Biochemistry, Leibniz Institute Of Plant Biochemistry (IPB), Halle, Germany*

Minimum Information (MI) standards are sets of guidelines for reporting investigations in a manner ensuring research reproducibility. They provide the framework to report not only the data, but also its context. They started in biology, while the field of chemistry has lacked its own autonomous, discipline-specific MI standards.

The German National Research Data Infrastructure for chemistry NFDI4Chem has stepped forward to catalyse the digitisation of chemical research by providing and supporting Electronic Laboratory Notebooks (ELN)s, data repositories, tools and standards. This initiative shifted the requirement from traditional reporting standards toward ones specialised for digitalised chemistry. Consequently, a primary objective of NFDI4Chem is the development of the Minimum Information about a Chemical Investigation (MIChI) framework. MI standards ensure experimental reproducibility and play a critical role in data harmonisation and integration by emphasising the provision of data in a standardised, machine-readable format, thereby facilitating interoperability and seamless data transfer across the scientific community. Notably, despite its nomenclature, MIChI extends beyond strictly "minimum" requirements by implementing varying levels of obligation, distinguishing mandatory core metadata from optional, supplemental ones.

NFDI4Chem envisions the MIChIs as a foundational component within a comprehensive digital ecosystem. This architecture begins with platforms that capture fields essential for reproducibility, which are connected via shared metadata schemas and annotated with community-approved ontologies using the NFDI4Chem terminology service. Ultimately, these semantically enriched chemical metadata can be harvested by search services to facilitate the construction of chemistry knowledge graphs (KG).

Building upon the established MIChI framework we used for NMR, UV-Vis, and MS, we are extending the initiative to cover Raman spectroscopy. This module aligns with the previous ones by capturing metadata across four sections: sample characteristics, instrumentation, acquisition parameters, and data processing. To ensure semantic interoperability, each metadata requirement is defined with controlled vocabulary (CV) terms. Where established CVs are unavailable, we use expert-vetted free-text definitions. The same applies for accepted values of the properties. A critical final phase of the MIChI development involves rigorous consultation with domain experts to ensure broad community acceptance, a milestone we aim to achieve through collaborative engagement at the International Conference on Raman Spectroscopy (ICORS).

Keywords: Minimum Information, Metadata, Standards, Guidelines, Schemas

[Abstract:0175] [Biology/Biomedicine]

Non-Destructive Qualitative Analysis of Locusts Using Raman Spectroscopy: A Novel, Non-Invasive Method for Species Identification, Biochemical Characterization, and Pest Management Applications without Sample Damage

***Anam Zulfiqar*, Jervee Punzalan, Yasmin Gadde, Daniel Mckenzie, Alaa El Din Bekhit, Keith Godon**

Dodd walls Centre and Department of Chemistry, University of Otago, New Zealand

Growing worldwide interest in insects, such as edible locusts, as a sustainable alternative protein source. To assess their composition and verify product authenticity, we need quick, reliable analytical methods.

In this research, Fourier Transform Raman (FT-Raman) spectroscopy coupled with principal component analysis was applied to investigate the chemical composition of locust samples. The objective was to differentiate between farm-raised and wild locusts using spectral features. FT-Raman spectra were collected using a 1064 nm Nd: YAG laser with a liquid nitrogen-cooled germanium detector. We collected Raman measurements from locust material and lipid extracts.

The Raman spectra showed distinct molecular features characteristic of lipids and fatty acids. Raman bands in the high-wavenumber region correspond to lipid chain vibrations. A band at approximately 3012 cm^{-1} was assigned to unsaturated fatty acids, while multiple features in the fingerprint region further confirmed the presence of fatty acid structures within the locust tissues. Principal component analysis of the data showed a clear difference between farmed and wild locust, suggesting that diet and environment affect their composition.

FT-Raman spectroscopy is a non-destructive method for characterizing edible insects, such as locusts. It can help monitor food quality and assess nutrition.

Keywords: Vibrational spectroscopy, locust, edible insects, fatty acids, chemometrics, principal component analysis (PCA)

[Abstract:0178] [SERS/TERS/Plasmonics]

SERS-based Acoustofluidic Platform for Rapid and Sensitive Bacterial Enrichment and Detection

Kyubin Kwon*, *Jaebum Choo

Department of Chemistry, Chung-Ang University, Seoul, South Korea

Sepsis is a life-threatening condition triggered by various pathogens, including *Escherichia coli* (*E. coli*). Early identification of the causative agent is critical, as the risk of mortality increases by up to 9% with each hour of delayed treatment. Conventional diagnostic methods rely on blood culture and molecular diagnostic methods; however, blood culture is time-intensive, while molecular methods require extensive sample processing, such as cell lysis and nucleic acid amplification. Here, we present a surface-enhanced Raman scattering (SERS)-based acoustofluidic chip for rapid and sensitive bacterial detection without lysis or washing steps. In this system, *E. coli* cells were labeled with SERS nanotags and introduced into a microfluidic channel, where two sequential processes occur within a single chip: (i) acoustically driven enrichment of labeled bacteria and (ii) standing surface acoustic wave (SSAW)-based separation of labeled *E. coli* from unbound SERS nanotags. This integrated microdevice enables rapid, on-chip bacterial detection within minutes by coupling enrichment, separation, and SERS-based identification in a single, lysis-free platform.

Keywords: Surface-enhanced Raman scattering (SERS), Acoustofluidic chip, Biosensor, Surface acoustic wave (SAW), Bacteria

[Abstract:0183] [SERS/TERS/Plasmonics]

Multimodal sensing of monosaccharides by molecular chirality- and identity-specific SERS responses of aromatic amino acids

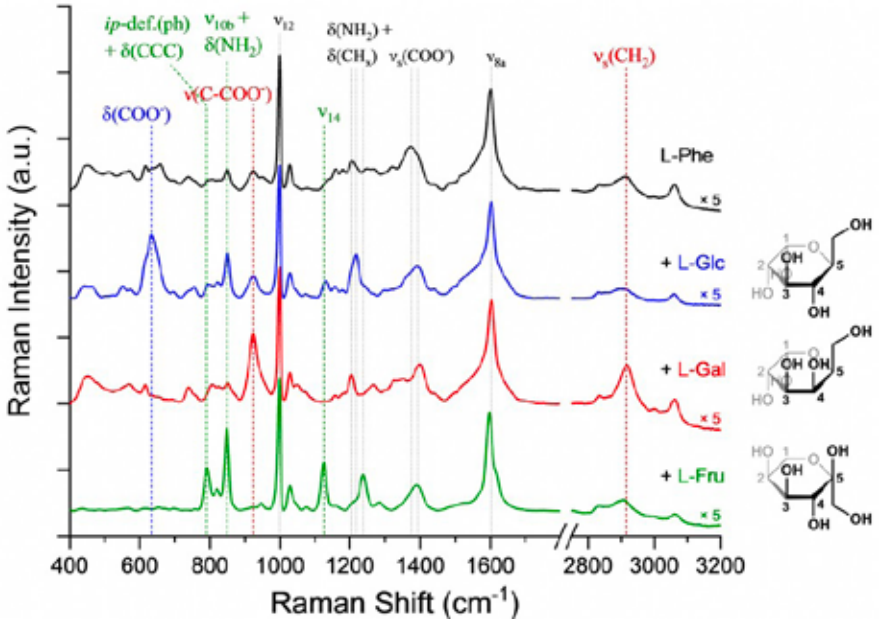
***Daedu Lee*, Jaehwan Jung, Yoonsoo Pang**

Department of Chemistry, Gwangju Institute of Science and Technology, Gwangju 61005, Republic of Korea

Chiral sensing is crucial in many disciplines including biochemistry and pharmacology since chiral-selective intermolecular interactions govern many biological and physiological processes. Recently, surface-enhanced Raman scattering (SERS) has attracted significant attention as a promising analytical technique for chiral sensing owing to its extremely high sensitivity and molecular fingerprinting capability. Enantioselective molecular interactions between target analytes and reporters induce characteristic changes in the SERS spectra of the reporters, enabling the identification of the chirality and identity of the target analytes. However, the chirality- and identity-specific SERS responses remain insufficiently understood, and these approaches have rarely been extended to biological systems containing multiple chiral species. In this study, we explored the sensing of the chirality and identity of monosaccharides using SERS of the reporters, phenylalanine (Phe) and tyrosine (Tyr) on gold nanoparticles. The SERS spectral changes of Phe occurred only upon addition of monosaccharides sharing the same chirality as Phe, which further depended on the molecular identity of each monosaccharide. As shown in Figure 1, glucose enhanced the $\delta(COO^-)$ mode in the Phe SERS, indicating changes in the surface adsorption of Phe via the carboxylate from bi- to monodentate binding [*Anal. Chim. Acta* 2024, 1330, 343290]. In contrast, galactose enhanced the ν(C-COO^-) and aliphatic CH2 stretching modes, while fructose induced enhanced lower-symmetric phenyl modes along with the disappearance of $\delta(COO^-)$ mode. The sensing of the chirality and identity of monosaccharides was also implemented using Tyr as a reporter under chirality-matching conditions, although the overall SERS spectral responses differed somewhat from those of Phe. The chirality- and identity-specific SERS spectral changes of Phe and Tyr enabled quantitative multimodal sensing of monosaccharide mixtures with principal component analysis and constrained least-squares optimization, demonstrating the potential of Phe and Tyr SERS as novel multimodal platforms for complex biological systems.

Keywords: Chirality, Surface-enhanced Raman scattering, Monosaccharides, Phenylalanine, Tyrosine

Figure 1. SERS spectra of L-phenylalanine (Phe) on gold nanoparticles without monosaccharides, and with the addition of L-glucose (Glc), L-galactose (L-Gal), and L-fructose (L-Fru).



[Abstract:0184] [Biology/Biomedicine]

Raman and Photoluminescence Imaging of Intracellular Localization of PEGylated Carbon Quantum Dots in Stem Cells

***Hyunhee Song*[1], *Eunsung Lee*[2], *Heesuk Rho*[2], *Hoon Jang*[3]**

[1]*Department of Biology, Jeonbuk National University, Jeonju, Republic of Korea*
[2]*Department of Physics, Research Institute for Materials and Energy Sciences, Jeonbuk National University, Jeonju, Republic of Korea*
[3]*Department of Life Sciences, Jeonbuk National University, Jeonju, Republic of Korea*

PEGylated carbon quantum dots (PEG-QDs) are promising nanomaterials for bioimaging and therapeutic applications. Understanding their effects on stem cells requires spatial characterization of how internalized quantum dots distribute within cells and induce biochemical redistribution. In this study, we performed Raman and photoluminescence (PL) mapping to characterize the intracellular localization of PEG-QDs and the associated biochemical changes in MC3T3-E1 pre-osteoblast stem cells. Label-free measurements were conducted on individual cells cultured on a SiO2/Si substrate, enabling simultaneous visualization of nanoparticle distributions and molecular compositions. PL mapping revealed enhanced PEG-QD signals predominantly in the perinuclear region. Raman spectroscopic mapping was further performed on the same samples to correlate PEG-QD distributions with lipid/membrane-related structures. Spatial correlation analysis showed that PEG-QD-enriched areas partially overlapped with protein-dense regions and membrane-related spectral features. These findings suggest preferential localization of PEG-QDs within membrane-dense perinuclear regions, potentially corresponding to endoplasmic reticulum–associated or vesicle trafficking regions. At higher exposure conditions, spectral alterations in the perinuclear membrane region were observed. These spectroscopic changes were consistent with independent biological data, indicating a correlation between localized biochemical redistribution and cellular stress responses. Overall, the simultaneous Raman and PL study enables spatially resolved investigation of nano–bio interactions by linking intracellular nanoparticle distribution with subcellular biochemical organization. This spectroscopy-based approach provides an integrative platform for analyzing organelle-proximal responses in stem cell systems.

*This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (No. 2021R1C1C1011346) and the G-LAMP Program of the NRF grant funded by the Ministry of Education (Grant No. RS-2024-00443714).

Keywords: Carbon quantum dot, Stem cell, Raman spectroscopy, Photoluminescence

[Abstract:0189] [SERS/TERS/Plasmonics]

Combined SERS and Chemometric Analyses of Blood Plasma and Bone Marrow Towards the Pediatric Leukemia Biomarkers Detection

***Aneta Aniela Kowalska*[1], *Patrycja Wiewiórowska*[1], *Magdalena Wołowiec*[2], *Marta Czaplicka*[1], *Sylwia Berus*[1], *Mateusz Pielach*[1], *Pawel Laguna*[2], *Agnieszka Kamińska*[1]**

[1]*Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland*
[2]*Department and Clinic of Oncology, Pediatric Hematology, Clinical Transplantology and Pediatrics, Medical University of Warsaw, Warsaw, Poland*

Leukemia is a heterogeneous group of hematologic malignancies characterized by the abnormal and uncontrolled proliferation of immature white blood cells in the bone marrow and peripheral blood. This malignant process originates in the bone marrow, where blood cells are normally produced, and leads to a disruption of hematopoiesis. In children, the two primary types of leukemia are acute and chronic; however, pediatric cases predominantly consist of acute leukemias, specifically acute lymphoblastic leukemia (ALL) and acute myeloid leukemia. Among these, ALL is the most common pediatric cancer, accounting for approximately 80% of leukemia cases in children. Conventionally used medical techniques for ALL recognition are most effective when performed on bone marrow samples, which require an invasive and often painful procedure, posing physical and emotional challenges for pediatric patients.

Therefore, we propose the surface-enhanced Raman spectroscopy (SERS) as a label-free analytical approach of blood plasma instead of bone marrow. We intended to compare obtained spectral data of bone marrow and blood plasma samples in a sense of possible new-tool differentiating based only on the blood. Samples were collected from pediatric patients at diagnosis, after induction therapy (33 days), and during consolidation (6 months) analyzed the partial least squares regression (PLSR) method. The distinct biochemical alterations were observed in spectra of leukemic and control samples and thus allow to recognize the marker bands. Moreover, used algorithm enabled separation of Control, Diagnosis, Induction, and Consolidation groups already in the first three latent variables.

To summarize the spectral differentiation is possible for blood plasma on a similar level of accuracy as for bone marrow samples, which allow the molecular-level spectral discrimination and in wider perspective give possibilities to use this method as therapeutic tool for ALL diagnosis, but also its monitoring of medical treatment.

Keywords: surface-enhanced Raman spectroscopy, acute lymphoblastic leukemia, chemometric analysis, partial least squares regression

[Abstract:0190] [SERS/TERS/Plasmonics]

Structural Characterization of Tel24 on Silver and Gold Nanoparticles Using SERS Spectroscopy

***Adriana Kenđel*, Klara Popović, Petra Petrović Popović, Snezana Miljanic**

Department of Chemistry, University of Zagreb Faculty of Science, Zagreb, Croatia

G-quadruplexes (G4s) are non-canonical secondary structures of nucleic acids formed by guanine-rich sequences. In living cells, they are involved in a range of essential biological processes. Considerable attention has been devoted to their role in telomere biology. The G-rich 3′ overhang of telomeres, composed of tandem TTAGGG repeats, can adopt G-quadruplex conformations that inhibit telomerase activity - an enzyme overexpressed in numerous cancer types and critically implicated in the uncontrolled proliferation of malignant cells. Accordingly, there is a clear need for analytical approaches capable of detecting and characterizing structural changes in G-quadruplexes under aqueous conditions that closely resemble the physiological environment, thereby facilitating a more comprehensive understanding of their mechanism of action. Surface-enhanced Raman scattering (SERS) spectroscopy is a highly sensitive vibrational spectroscopic technique that enables structural characterization of low-concentration analytes in the vicinity of nanostructured metal surfaces. Due to its high sensitivity and its ability to provide molecularly specific fingerprint spectra in aqueous media, SERS is particularly well suited for bioanalytical applications. To assess the suitability of SERS for the structural characterization of oligonucleotides capable of forming G4 structures, silver and gold colloidal nanoparticles were employed as metallic substrates. The nanoparticles were synthesized by chemical reduction of metal salts with sodium citrate. Subsequently, one portion of the prepared colloids was aggregated with magnesium sulfate, while the other was functionalized with thiol-modified telomeric DNA sequence d[$(TTAGGG)_4$] (Tel24). All SERS measurements for the Tel24 oligonucleotide were performed using 785 nm excitation. SERS spectra of Tel24 recorded on freshly prepared and aggregated nanoparticles were compared with spectra obtained from oligonucleotides-functionalized metal nanoparticles. Detailed analysis of band positions and relative intensities in the recorded SERS spectra demonstrated that surface modification of colloidal silver and gold nanoparticles significantly affects the stacking and orientation of the oligonucleotide at the metal surface. Aggregation of silver nanoparticles resulted in localized electromagnetic “hot spots” associated with enhanced inelastic scattering, providing the most suitable substrate for structural characterization of the Tel24 oligonucleotide.

Keywords: colloids, SERS, Tel24, G-quadruplexes

Posters

[Abstract:0191] [SERS/TERS/Plasmonics]

SERS Plasmonic Structure for Biomedical Applications

***Ariadna B. Nowicka*[1], *Aneta Aniela Kowalska*[1], *Ida Dominika Wiśniewska*[1], *Tomasz Szymborski*[1], *Zuzanna Gronkiewicz*[2], *Wojciech Kukwa*[2], *Magdalena Data*[2], *Agnieszka Kamińska*[1]**

[1]*Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland*
[2]*Czerniakowski Hospital, Medical University of Warsaw, Warsaw, Poland*

Surface-enhanced Raman spectroscopy (SERS) is a non-destructive, rapid vibrational spectroscopy technique with hight sensitivity down to single molecular level. It provides a fine molecular fingerprint, allowing for direct identification of target analytes. This is achieved through the amplification of electromagnetic fields (up to 108) and/or the creation of charge-transfer states (up to 103) between the chemisorbed analyte molecule and the SERS-active platform. It can be used to detect chemical analytes at low concentrations (10–12 mol·dm^{-3}), a variety of biological systems, such as bacteria, circulating tumour cell etc. and also as a diagnostic tool for environmental and biomedical analysis (Biosensors 2019, 9, 2, 57; Photonics, 2025, 12, 8, 809).

SERS platforms are usually made of metals like silver, gold or copper in a form of nanostructured substrates, colloidal metal nanoparticles, lithographically fabricated nanostructures, core–shell nanostructures, as well as flexible and polymeric substrates and semiconductor-based SERS platforms (Analytica Chimica Acta, 2024, 1296, 342291; Chemosensors. 2023, 11, 8, 427).

In this study, we will present various types of SERS active platforms (e.g. based on silicon modified on the surface by laser ablation and covered with SERS-active metal, metal nanoparticles) for detection of various cell lines eg. A64-CLS, HeLa and compere of using micro and hand handle Raman equipment for biomedical applications.

Acknowledgements: This work was supported by the National Science Centre Poland OPUS 28 no 2024/55/B/ST4/01457.

Keywords: Surface-Enhanced Raman Scattering (SERS), SERS substrates, biomedical applications,

[Abstract:0192] [Materials]

Strain-Dependent Raman Signatures of Interlayer Phonons in Few-Layer MoS2

Daekwon Lee, Heesuk Rho

Department of Physics, Research Institute for Materials and Energy Sciences, Jeonbuk National University, Jeouju, Republic of Korea

Strain engineering is one of the most effective approaches for tuning the physical properties of two-dimensional (2D) materials. In layered 2D semiconductors, uniaxial strain can modify the band structure, lattice symmetry, and vibrational characteristics, thereby providing a practical route for controlling optical and electronic responses in sensors and optoelectronic devices. Although strain-induced changes in intralayer phonons have been widely studied, the thickness dependence of strain sensitivity and the behavior of *interlayer* vibrational modes remain less well understood. In this work, we investigate the strain-dependent Raman response of few-layer MoS_2 with layer numbers ranging from 2 to 5. Under uniaxial tensile strain, the originally hexagonal lattice becomes distorted, leading to anisotropic restoring forces along and perpendicular to the strain axis. We observe that this symmetry lowering causes the doubly degenerate intralayer Eg phonon to split into two singlets at a strain of approximately 0.4%, while the A1g phonon exhibits a clear redshift. Furthermore, the interlayer shear and layer breathing modes show systematic wavenumber shifts with increasing strain, accompanied by splitting of the shear modes. As the thickness increases, the strain-induced A1g phonon and Eg phonon shifts become progressively weaker. From these results, we extract the Grüneisen parameters and shear deformation potentials, both of which decrease with increasing layer number, indicating reduced phonon sensitivity to strain in thicker MoS_2. We further performed polarized Raman measurements on MoS_2 under 1% uniaxial tensile strain. Interestingly, the two singlet modes originating from the Eg and shear modes exhibit strong polarization anisotropy with orthogonal characteristics in their intensity profiles. By comparing the measured polarization dependence with calculations based on the Raman polarization selection rules, we determine the angular offset between the strain direction and the crystal zigzag axis without requiring additional structural characterization. These results demonstrate that Raman spectroscopy provides a powerful tool for probing phonon symmetry breaking and identifying crystal-axis orientation in strained 2D materials.

[This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (Grant No. RS-2025-23324133) and the G-LAMP Program of the NRF grant funded by the Ministry of Education (Grant No. RS-2024-00443714).]

Keywords: MoS2, Uniaxial strain, Interlayer phonon, Raman spectroscopy

[Abstract:0205] [Biology/Biomedicine]

Advancing SERS based Therapeutic Drug Monitoring for Point of Care Monitoring of Methotrexate

***Amalie Løvind Årsten*[1], *Yaman Göksel*[1], *Gohar Soufi*[1], *Martyna Anna Pytlarz*[1], *Roman Slipets*[1], *Raheel Altaf Raja*[2], *Kjeld Schmiegelow*[2], *Anja Boisen*[1]**

[1]*Department of Health Technology, Technical University of Denmark, Kgs. Lyngby, Denmark*
[2]*Department of Paediatrics and Adolescent Medicine, Rigshospitalet University Hospital, Copenhagen, Denmark*

Therapeutic drug monitoring (TDM) of methotrexate (MTX) is critical in pediatric oncology to ensure treatment efficacy and avoid toxicity [Cancers (2026), 18(1), 124; Cancer Chemother Pharmacol(2025), 95, 33]. Conventional methods require centralized laboratory infrastructure and extended turnaround times. Surface-enhanced Raman scattering (SERS) offers a rapid and label-free alternative but faces challenges with matrix effects and automation. In this work we target these challenges by a novel SERS based approach with an integrated centrifugal microfluidic disc combined with microextraction by packed sorbent (MEPS).

Silver coated nanopillar substrates imbedded within the disc were used for analysis by controlled analyte deposition through centrifugal microfluidics. MEPS were used for its compatibility with automation and to reduce sample matrix variations. The collected spectral SERS data were analyzed using multivariate methods such as partial least square regression (PLSR) for quantification. Performance was assessed for pediatric leukemia patient samples spiked with MTX and samples collected 24 hours after MTX treatment, including limit of detection (LoD), limit of quantification (LoQ), linear range and relative standard deviation (RSD). Results were compared to benchmark reference methods. A schematic presentation of the method implemented in this work is presented in Figure 1.

Our method enabled automatic pre-treatment and measurement of the samples with reliable detection of MTX within a clinically relevant therapeutic range of 15-200μM with LoD of 5μM and average RSD of 6%. Matrix effects were minimized by MEPS pre-treatment and analysis, improving quantification reliability and clinical application potential. Multivariate modelling allowed robust MTX quantification while compensating for residual matrix background while consistent trends were observed compared to reference methods.

Combining automated sample pre-treatment with integrated SERS detection provides a promising step towards rapid and reliable point of care therapeutic drug monitoring.

Keywords: SERS, Therapeutic Drug Monitoring, Methotrexate

Figure 1. Procedure of assay of methotrexate quantification implemented in this work

[Abstract:0209] [Biology/Biomedicine]

Immune Monitoring by Raman Spectroscopy from Acute Inflammation to Stress-induced Dysfunction

Anuradha Ramoji[1], Klaudziya Kamiak[3], Tze Ching Yeo[2], Hulya Yilmaz[2], Aikaterini Pistiki[2], Thomas Bocklitz[2], Andreas Stallmach[3], Christian Puta[4], Juergen Popp[2], Philipp A. Reuken[3]

[1]Institute of Physical Chemistry and Abbe Center of Photonics, Friedrich Schiller University Jena, Jena, Germany
[2]Leibniz Institute of Photonic Technology, Jena, Germany
[3]Department for Internal Medicine IV, Jena University Hospital, Jena, Germany
[4]Department of Sports Medicine and Health Promotion, Friedrich-Schiller-University Jena, Jena, Germany

Raman spectroscopy is an emerging, label-free technology that enables phenotyping of immune cells based on their intrinsic molecular composition (Anal.Chem. 2012,84,12,5335–5342). In an initial prospective clinical study, we demonstrated that circulating leukocytes from patients with sepsis display distinct spectral patterns consistent with immune activation and inflammatory stress. These findings established the feasibility of using Raman-based profiling to detect clinically relevant immune cell states directly from patient samples (Crit Care Explor. 2021,12;3(5):e0394). Subsequent longitudinal studies expanded upon this approach to encompass acute and persistent inflammatory conditions, including viral and non-viral sepsis. The study revealed dynamic spectral changes in leukocytes during disease progression and recovery, indicating Raman signatures can track evolving immune responses. Notably, the immune cell profiles not only distinguished between distinct sepsis etiology but also reflected temporal adaptation and ongoing immune dysregulation (Biotechnology Journal 20,no.9 (2025):20,e70105). We are now applying Raman spectroscopic analysis to peripheral blood mononuclear cells collected before and 24h after controlled physical exertion (STS-test) in individuals with post-infectious exertion intolerance. Preliminary data suggest that affected individuals exhibit distinct immune cell signatures at baseline compared with healthy controls, with further divergence following exertion. These stress-associated spectral shifts are indicative of altered immune responsiveness and reduced adaptive capacity. It is important to note, the presence of heterogeneous response patterns within the cohort suggests the existence of biologically distinct subgroups. The collective findings of this research demonstrate the potential of Raman spectroscopy for the sensitive monitoring of immune cell state changes across a range of physiological conditions, including acute inflammation, persistent immune alteration, and stress-related dysfunction. The platform under consideration functions as a non-destructive and reproducible system for immune phenotyping. It provides coherent framework for the investigation of immune adaptation and maladaptation across diverse clinical contexts. In addition, it supports the development of patient stratification strategies based on underlying immune response in complex inflammatory conditions.

Acknowledgement: This research was supported by funding from the Deutsche Gesellschaft ME/CFS (№007622).Federal Ministry of Research,Technology and Space (BMFTR) funded project BioSig-PEM (FKZ:01EJ2408B),SARS-CoV-2Dx (FKZ:13N15745) and within the funding program Photonic Research Germany (LPI-BT1-FSU,FKZ13N15466;LPI-BT2-IPHT,FKZ13N15704), and is integrated into the Leibniz Center for Photonics in Infection Research.

Keywords: Myalgic encephalomyelitis/chronic fatigue syndrome, Immune cells, PBMC, Raman spectroscopy

[Abstract:0213] [Theory/Computation]

Distilled Nyström embeddings enable fast single-cell Raman identification

***Ario Jafari*[1], *Pardis Jayervand*[2], *Daniel Aili*[1], *Thomas Ederth*[1]**

[1]*Division of Biophysics and Bioengineering, Department of Physics, Chemistry and Biology, Linköping University, SE-58183 Linköping, Sweden.*
[2]*Reasearch and Innovation Center, Livogen Pharmed Co., 1417755358Tehran, Iran.*

Single-cell Raman spectroscopy can separate microbial species without labels, but the most accurate classifiers often rely on nonlinear kernels whose cost becomes prohibitive when models must be re-trained many times (e.g., repeated cross-validation) or deployed on resource-limited CPUs. We propose an explicit, distilled embedding pipeline that retains the discriminative power of a Nyström kernel model while replacing kernel evaluation at test time with simple linear algebra.

Each spectrum x is preprocessed $z \in R^d$ (Savitzky–Golay smoothing, asymmetric least-squares baseline correction, and L_2 normalization), projected to k principal components using fold-contained PCA ($u \in R^d$), and passed to a *(I)* Nyström teacher built from m landmark spectra (rank r) to produce K-class score vectors $s_T(x) \in R^K$. A compact *(II)* student matches the teacher via score-based distillation: the PCA scores are expanded once by a fixed random feature map $h \in R^p$ and a multi-output ridge readout $s_S(x) \in R^K$ is trained on a convex blend of hard labels and temperature-softened teacher probabilities $y^{\wedge}$. We evaluate the method on a low-SNR single-cell Raman benchmark (1 s integration) containing seven clinically relevant species (1750 spectra). Using repeated stratified 10-fold cross-validation with PCA k=49 and a fixed Nyström teacher (m=160 landmarks, rank r=60), a 500-trial sweep over student width, ridge regularization, and distillation temperature maps the accuracy–latency–memory trade space (Fig. 1a). The best trade-off configuration achieves 91.31±1.23% accuracy at 0.002 ms/spectrum inference and 0.91 KB/spectrum working-set memory. The confusion matrix (Fig. 1b) is strongly diagonal, with residual errors dominated by *Staphylococcus epidermidis* versus *Staphylococcus aureus*.

Keywords: Raman spectroscopy, single-cell analysis, bacterial identification, kernel approximation, efficient inference

Equation

$$x \xrightarrow{\text{preprocess}} z \in \mathbb{R}^d \xrightarrow{\text{PCA}(k)} u \in \mathbb{R}^k$$

$$(I)\ u \in \mathbb{R}^k \xrightarrow{\text{Nyström } (m,r)} s_T(x) \in \mathbb{R}^K$$

$$(II)\ u \in \mathbb{R}^k \xrightarrow{\phi(\cdot)} h \in \mathbb{R}^p \xrightarrow{\text{ridge}} s_S(x) \in \mathbb{R}^K \xrightarrow{\text{decision}} \hat{y}$$

Figure 1

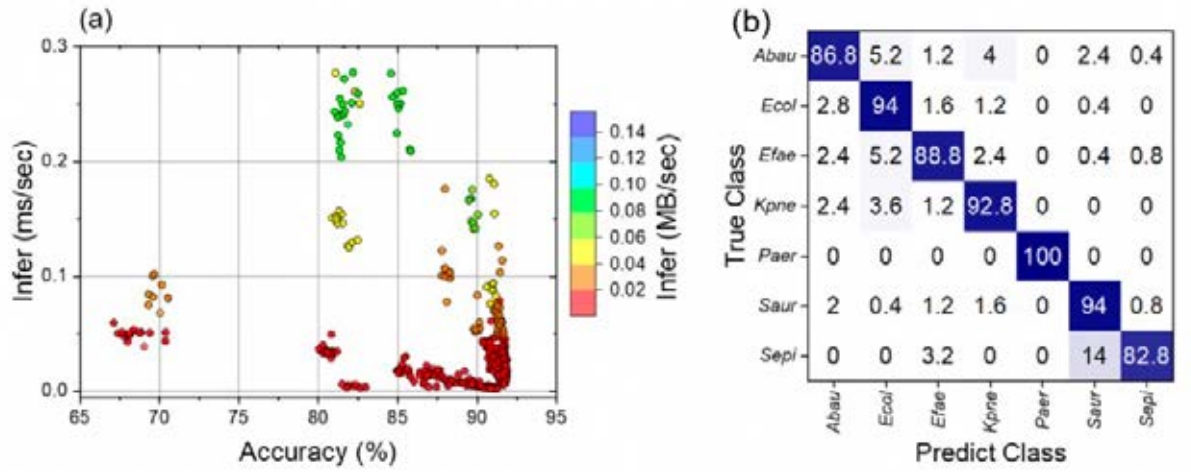


Figure 1. (a) 500-trial sweep on dataset showing accuracy versus inference latency. (b) Row-normalized confusion matrix (%) for the best trade-off student configuration. Abbreviations: Abau, Acinetobacter baumannii; Ecol, Escherichia coli; Efae, Enterococcus faecalis; Kpne, Klebsiella pneumoniae; Paer, Pseudomonas aeruginosa; Saur, Staphylococcus aureus; Sepi, Staphylococcus epidermidis.

[Abstract:0218] [SERS/TERS/Plasmonics]

Flexible Silver-Coated Gold Nanoparticles Loaded Graphene Textiles for Broad-Spectrum In-Situ Detection of Pesticide Residues

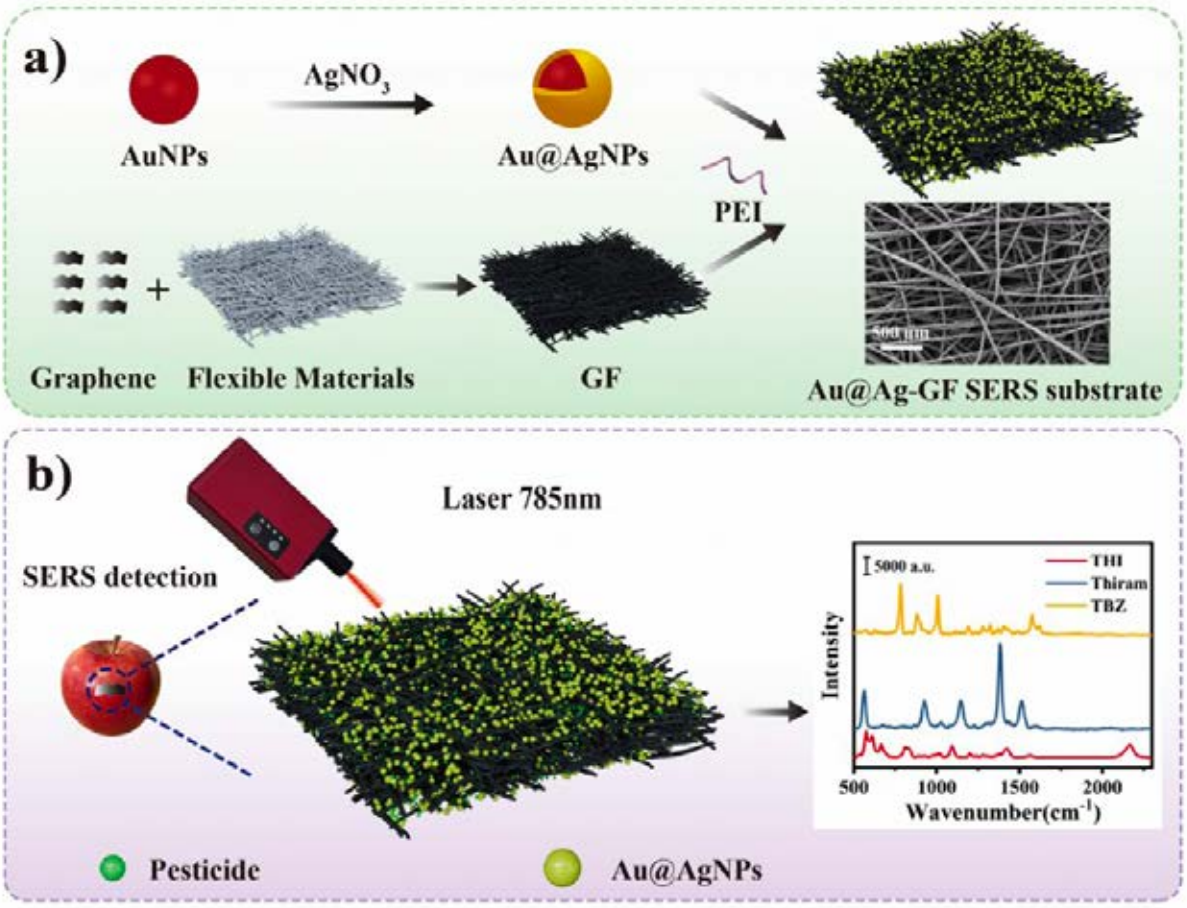
***Sujia Jiao*[1], *Long Wu*[2], *Jyothi B. Nair*[1], *Guobin Jia*[1], *Jonathan Plentz*[1], *Jürgen Popp*[1], *Dana Cialla May*[1]**

[1]*Leibniz Institute of Photonic Technology, Jena, Germany*
[2]*School of Food Science and Engineering, Hainan University, Haikou, PR China*

The widespread use of various pesticides poses potential hazards to human health and ecosystems, necessitating rapid, versatile, and on-site screening methods. In this study, we developed a highly sensitive and flexible surface-enhanced Raman scattering (SERS) substrate (Au@Ag-GF) by decorating a graphene-loaded polypropylene textile with gold-silver core-shell nanoparticles (Fig. 1a). This design leverages the synergistic effect of the graphene framework and dense, uniform nanoscale hotspots, ensuring exceptional sensitivity, batch consistency, and stability. Crucially, we applied this versatile substrate directly to the detection of a panel of commonly used pesticides. For the neonicotinoid insecticide thiacloprid (THI), quantitative analysis was achieved using its Raman silent zone peak at 2170 cm-1. Furthermore, the sensor's capability was successfully extended to the fungicides thiram and thiabendazole (TBZ), exhibiting distinct spectral recognition and clear target identification. Coupled with a handheld Raman spectrometer, a simple wipe sampling method facilitated direct in-situ detection on irregularly curved surfaces such as apple skin. This approach successfully identified trace residues of THI, thiram, and TBZ (Fig. 1b). This flexible substrate, combined with portable Raman instrumentation, provides a highly sensitive, reproducible, and robust analytical platform for the multiplexed, on-site monitoring of pesticide residues in food safety applications.

Keywords: Surface-enhanced Raman scattering, flexible substrate, pesticide residues, handheld Raman spectrometer, food safety

Figure 1. Schematic of the construction of Au@Ag-GF flexible SERS substrate and its application for multiplex detection of pesticides including THI, Thiram, and TBZ.



[Abstract:0221] [SERS/TERS/Plasmonics]

Towards an Optofluidic Platform for Bioanalysis Based on SERS

***Anant Mantha*[1], *Jérémy Bell*[2], *Knut Rurack*[2], *Janina Kneipp*[1]**

[1]*Department of Chemistry, Humboldt Universität zu Berlin, Berlin, Germany*
[2]*Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany*

Surface Enhanced Raman Scattering (SERS) is an optical probing technique that is highly selective and sensitive. Integrating SERS with microfluidics miniaturises the sample environment while allowing control of environmental parameters of the analyte and the plasmonic SERS substrate. Moreover, it allows for applications of SERS involving sample volumes in the µL-pL regime, thereby making it suitable for bioanalytical applications.

Direct usage of nanoparticles in the sample solution can cause a range of issues leading to undesirable memory effects. Here, we report the use of removable PDMS inserts with plasmonic nanostructured surfaces that improve the reusability of the microfluidic channel as they can be replaced post measurement. The inserts also introduce a relatively large surface that can be sampled and can improve the reproducibility of the measurements. We will discuss the fabrication and characterization of the plasmonic nanostructured surfaces for the PDMS inserts, present their surface morphology, plasmonic properties as well as their performance as SERS substrates. Moreover, the spectra of potential non-resonant analytes will be discussed.

Keywords: SERS,Optofluidics,Bioanalysis

Posters

[Abstract:0228] [SERS/TERS/Plasmonics]

A SERS-Integrated Vertical-Flow Paper Chip with Gold-Coated Cellulose Fiber Substrates for Sensitive Biomarker Detection

Ji Qi, Jaebum Choo

Department of Chemistry, Chung-Ang University, Seoul, South Korea

Paper-based analytical devices offer great promise for point-of-care testing (POCT) due to their low cost, portability, and intrinsic fluid actuation via capillary flow. However, achieving quantitative optical analysis on paper remains challenging: colorimetric assays suffer from limited sensitivity, while fluorescence-based methods often experience signal quenching and attenuation within fibrous cellulose matrices. Surface-enhanced Raman scattering (SERS) provides an attractive solution to these constraints by enabling highly sensitive and quantitative optical detection. Here, we present a vertical-flow arrayed paper chip for SERS–based biomarker detection. The device features a multilayer vertical-flow structure that integrates sample loading, conjugate release, immunoreaction, and fluidic control into a compact paper-based architecture. The detection layer is produced through thermal vapor deposition, generating well-defined arrays of gold-coated cellulose fiber wells functionalized with capture antibodies. Upon target binding, analytes labeled with SERS nanotags are selectively retained within the detection layer. Strong electromagnetic hot spots formed between the nanotags and the gold-coated cellulose fiber surfaces yield substantial Raman signal enhancement. The recorded Raman intensities exhibit a clear linear correlation with analyte concentration. This integrated SERS-paper platform significantly improves sensitivity and quantitative precision, providing a robust approach for trace-level biomarker analysis in POCT and field-deployable diagnostics.

Keywords: SERS substrate, paper-based device, immunoassay, biomarker

[Abstract:0229] [SERS/TERS/Plasmonics]

Potential-Controlled Binding and Readout in an EC-SERS Aptamer Sensor for Rapid and Sensitive Thrombin Detection

***Yujin Cha*, Jaebum Choo**

Department of Chemistry, Chung-Ang University, Seoul, South Korea

In aptamer-functionalized substrates, conventional surface immobilization often suffers from diffusion-limited target binding and reduced sensitivity due to random probe orientations and inefficient localization within plasmonic hotspots. Here, we report an electrochemical surface-enhanced Raman spectroscopy (EC-SERS) platform that enables rapid and sensitive thrombin (a key biomarker related to the blood coagulation cascade) detection by dynamically modulating aptamer conformation and signal localization through potential control. The sensing substrate, composed of a gold nano-popcorn structure rich in plasmonic hotspots, ensures reproducible and enhanced Raman signals. A cDNA–thrombin binding aptamer (TBA15) duplex was immobilized on the surface with 6-mercapto-1-hexanol (6-MCH) serving as a blocking layer. During target recognition, application of a negative potential induces an upward orientation of the DNA duplex, promoting rapid and efficient thrombin binding via enhanced electrostatic attraction between the aptamer and the positively charged protein. Upon thrombin–aptamer complex formation, the Cy5-labeled aptamers dissociate from their cDNA anchors, leading to a decrease in surface-bound Cy5 Raman reporters—thus enabling a quantitative signal-off response. For signal readout, application of a positive potential drives the remaining Cy5-labeled aptamers toward the gold surface, thereby localizing them within plasmonic hotspots and thereby improving detection sensitivity.

Keywords: Electrochemical surface-enhanced Raman scattering (EC-SERS), aptamer, thrombin detection, gold nano-popcorn substrate

[Abstract:0231] [SERS/TERS/Plasmonics]

A Rapid and Highly Sensitive One-Pot Detection Assay for Lung Cancer ctDNA Using a SAW-Enhanced CRISPR-SERS Platform

***Mina Shin*, Jaebum Choo**

Department of Chemistry, Chung-Ang University, Seoul, Republic of Korea

The SHERLOCK (Specific High-sensitivity Enzymatic Reporter unLOCKing) system, based on CRISPR/Cas, enables highly sensitive and specific detection of trace nucleic acids (NAs) via fluorescence readout generared by quenched probe cleavage. However, conventional fluorescence-based SHERLOCK assays are limited by diffusion-controlled reaction kinetics at low NA concentrations, which makes it difficult to detect trace targets within a short assay time. To address this limitation, isothermal pre-amplification (e.g., RPA, RT-RPA) is typically required, thereby compromising assay simplicity and speed. Here, we introduce a surface acoustic wave (SAW)-induced microwell chip integrated with a surface-enhanced Raman scattering (SERS) assay for rapid and sensitive detection of circulating tumor DNA (ctDNA) in lung cancer liquid biopsy. SAW-induced acoustic streaming in the microwell chip markedly accelerates CRISPR-Cas12a target recognition and collateral cleavage, reducing the reaction time by more than six-fold without the need for NA amplification. Integration with a SERS-based assay further enables highly sensitive, one-pot detection of target nucleic acids within the microwell chip through Raman signal enhancement. This integrated SAW/CRISPR-SERS platform provides a rapid and highly sensitive ctDNA detection strategy, with strong potential for early cancer diagnosis via liquid biopsy.

Keywords: Surface-enhanced Raman Scattering (SERS), CRISPR-Cas12, circulating tumor DNA (ctDNA), surface acoustic wave (SAW), one-pot assay

[Abstract:0232] [Biology/Biomedicine]

Enhancing Isolate-Level Classification of *Klebsiella pneumoniae* through Data Fusion of Raman and FTIR Spectroscopy

María Gabriela Fernández-Manteca*[1], Adolfo Cobo[2], Domingo Fernández Vecilla[3], Nuria Valcárcel Fraile[4], Borja García García[1], Ana Sobrino Santos[1], Celia Gómez Galdós[1], José Francisco Algorri[2], Alain A. Ocampo-Sosa[5], Luis Rodríguez-Cobo[2]

[1]*Grupo de Ingeniería Fotónica, Universidad de Cantabria, Santander, Spain; Instituto de Investigación Sanitaria Valdecilla (IDIVAL), Santander, Spain.*
[2]*Grupo de Ingeniería Fotónica, Universidad de Cantabria, Santander, Spain; Instituto de Investigación Sanitaria Valdecilla (IDIVAL), Santander, Spain; Centro de Investigación Biomédica en Red en el área temática de Bioingeniería, Biomateriales y Nanomedicina (CIBER-BBN), Instituto de Salud Carlos III, Madrid, Spain.*
[3]*Servicio de Microbiología, Hospital Universitario Marqués de Valdecilla, Santander, Spain.*
[4]*Instituto de Investigación Sanitaria Valdecilla (IDIVAL), Santander, Spain.*
[5]*Servicio de Microbiología, Hospital Universitario Marqués de Valdecilla, Santander, Spain; Instituto de Investigación Sanitaria Valdecilla (IDIVAL), Santander, Spain; Centro de Investigación Biomédica en Red de Enfermedades Infecciosas (CIBERINFEC), Instituto de Salud Carlos III, Madrid, Spain.*

Accurate and rapid identification and classification of bacterial pathogens at the isolate level is a critical challenge in clinical microbiology and epidemiology. *Klebsiella pneumoniae*, a prominent opportunistic pathogen known for its varying resistance profiles and hypervirulent strains, requires robust characterization methodologies. While vibrational spectroscopic techniques, namely Raman and Fourier-transform infrared (FTIR) spectroscopy, have independently demonstrated significant potential for bacterial identification, both face inherent limitations in complex biological matrices when attempting precise isolate differentiation.

This study investigates a multimodal approach combining Raman and FTIR spectroscopy to improve the classification performance of *Klebsiella pneumoniae* at the isolate and phenotype levels (capsular serotypes K1, K2, K54 and K57). We compiled two extensive datasets containing +3000 spectra across 18 characterized isolates. A convolutional neural network (CNN) model was independently trained on each modality, achieving high accuracies (> 90% validation accuracy) at the phenotype level, but much lower accuracies at the isolate level. Raman is known for its high molecular specificity, but its application is inherently limited by weak signal scattering and high susceptibility to background autofluorescence and inter-experiment variability (batch effects). Conversely, while FTIR spectroscopy yields strong, repetitive signals reflecting bulk macromolecular composition (such as lipids and carbohydrates), it generates broader, overlapping absorption bands that limit its discriminative power for subtle, isolate-specific variations.

To leverage the complementary biochemical information provided by the distinct vibrational modes of each technique, we developed a data fusion framework. The methodology involves the normalization of Raman and FTIR spectra, followed by a randomized concatenation strategy within shared isolates to address dataset imbalances. The combined spectral representations are then analyzed using advanced deep learning architectures and cross-modal feature fusion algorithms.

Our preliminary findings indicate that the integration of FTIR (primarily capturing macromolecular composition like lipids and carbohydrates) and Raman (highly sensitive to specific molecular bonds like nucleic acids and proteins) provides a more comprehensive biochemical fingerprint. This fused dataset mitigates the misclassification

rates observed in isolated techniques, suggesting that multimodal vibrational spectroscopy, enhanced by explainable AI and chemometric analysis, constitutes a highly robust, non-invasive tool for the accurate screening and epidemiological tracking of *Klebsiella pneumoniae* isolates.

Keywords: Raman spectroscopy, FTIR, bacterial characterization, Klebsiella pneumoniae, data fusion, deep learning.

[Abstract:0234] [Novel Approaches]

The Effects of Structural Evolution on Hardness of SiCf/SiC Composites Studied by In-situ Raman Spectroscopy

Guofeng Cheng*, *Huiyang Wu

Shanghai Institute of Ceramics, Chinese Academy of Sciences

The degradation of the SiCf/SiC composites under oxidation environments was investigated by a new In-situ Raman spectroscopy technique. The results show that the relative vibration of Si and C atoms in protocells was inhibited in dry oxygen environment. Steam eliminated the inhibition of the relative vibration of Si-C atoms during high temperature oxidation process. In addition, the BN interface phase began to volatilize at 1000°C. The micro mechanical properties such as hardness and Young's modulus of the composites were further studied by nano indentation. Both hardness and Young's modulus decrease after oxidation. The fracture of Si-C bond leads to the deterioration of the mechanical properties, and water vapor intensified the fracture of Si-C bond, which accelerated the deterioration of the composites.

Keywords: SiCf/SiC composites, Hardness, Young's modulus, Wet oxidation, Raman spectroscopy

[Abstract:0240] [Biology/Biomedicine]

From 5'-GMP To G-Quadruplex: Raman Spectroscopy as a Quantitative Probe of Supramolecular Nucleotide Self-Assembly

***Lucia Ďuríšková*, Štěpán Jílek, Václav Profant**

Institute of Physics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

Mononucleotide G-quadruplexes (mG4) represent supramolecular assemblies formed by the self-association of guanine mononucleotides into stacked G-quartets stabilized by monovalent cations. These systems are considered simple analogues of G-quadruplex structures known from genomic DNA and have attracted interest in areas ranging from prebiotic chemistry to bionanotechnology. Their characterization commonly relies on techniques such as NMR or dynamic light scattering to probe aggregate formation and size distribution. We explore an alternative spectroscopic approach and employ Raman spectroscopy to monitor the mG4 self-assembly and to resolve the molecular species participating in the aggregation process.

In the present work, we investigate the self-assembly of guanosine-5'-monophosphate (5'-rGMP) in the presence of Na^+, K^+ and Li^+ ions, using concentration- and temperature-dependent Raman spectroscopy (Figure 1, a). Statistical deconvolution of the spectral series enables assignment of distinct Raman signatures to individual species: free 5'-rGMP, stacked GMP units, and stacked G-quartets (mG4) (Figure 1,b).

Using an association model tailored to the Raman spectral response that describes the stepwise formation of stacked monomers, G-quartets, and their further aggregation within an indefinite isodesmic framework, we extract quantitative insights into the self-assembly pathway, including the population distribution of distinct species and the effective size of the aggregates. The model further yields thermodynamic parameters (ΔH, ΔS, K) characterizing each step of the association process, with notable differences observed between the Na^+-, K^+- and Li^+-stabilized 5'-rGMP systems.

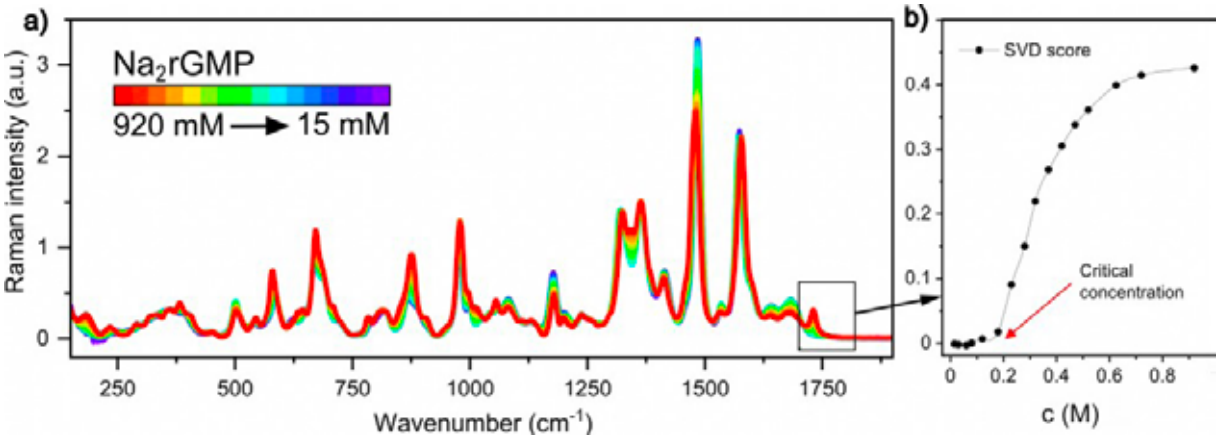
The findings are supported by complementary UV absorption and electronic circular dichroism (ECD) spectroscopy.

Our results offer a detailed spectroscopic characterization of supramolecular nucleotide self-assembly and demonstrate that Raman spectroscopy, combined with statistical analysis and association modelling, can unravel and quantify complex supramolecular equilibria.

Acknowledgements: This research was supported by SVV-2025-260832 from Charles University.

Keywords: Self-assembly, G-Quadruplex, GMP, Supramolecular Chemistry, Thermodynamics

Figure 1.



a) Raman spectra of Na2rGMP measured at concentrations ranging from 0.015 to 0.920 M. b) Singular Value decomposition score of mG4 Raman marker indicates aggregation at critical concentration.

[Abstract:0245] [Coherent Raman Imaging]

Investigating the Link Between Microplastic Intake and Lung Disease Using Raman Spectroscopy

***Emma Smith*[1], *Natalie Warren*[1], *Emily Sprague Klein*[1], *Sharon Rounds*[2], *Erica Herzog*[3]**

[1]*Chemistry, Brown University, Providence, United States of America*
[2]*Medicine & Laboratory and Pathology Medicine, Warren Alpert Medical School, Brown University, Providence, United States of America*
[3]*Medicine and Pathology, Yale School of Medicine, Yale University, New Haven, United States of America*

The growing prevalence of microplastics and nanoplastics (MNPs) in everyday life is a mounting global concern given how little is known about their short and long-term effects on human health. Due to the abundance of MNPs found in household products such as textiles, cosmetics, and kitchenware, as well as their use in industrial and agricultural processes, investigating links between MNPs and disease is essential. Previous studies have identified MNPs within a variety of human specimens including the brain, lungs, placenta, testes, and urine. Specifically exposure to MNPs was linked to interstitial lung diseases (ILD) in workers at a flocking factory in Rhode Island in 1995; however a definitive link between MNP uptake and disease initiation has yet to be established. Stimulated Raman scattering (SRS) microscopy is a powerful technique for label-free biomedical imaging and mapping due to its chemical specificity, lack of fluorescence background, and improved imaging speeds and contrast when compared to traditional spontaneous Raman spectroscopy. Here we employ SRS as well as traditional vibrational spectroscopic methods including micro-infrared and micro-Raman spectroscopies to map distributions and concentrations of MNPs within lung tissue samples, pairing characteristic spectral information to optical images. Such spectra can identify the presence of MNPs as well as vibrational signatures associated with fibrotic tissue, reactive oxygen species (ROS) generation, and other markers of ILD. We assess the concentrations and spatial distributions of MNPs found in age and sex-matched lung tissue sections to determine correlations between the presence of MNPs and fibrotic tissue. Overall, this work marks an effort towards establishing a link between MNP uptake and pulmonary disease, investigating the impact and mechanism of MNP effects on cellular function.

Keywords: Stimulated Raman Scattering, Microplastics, Lung Disease

[Abstract:0249] [Biology/Biomedicine]

Compact Hybrid SERS Platform Integrating Centrifugal Microfluidics and Automated Sample Preparation for Point-of-Need Therapeutic Drug Monitoring

***Roman Slipets*[1], *Yaman Göksel*[1], *Gohar Soufi*[1], *Martyna Anna Pytlarz*[1], *Amalie Løvind Årsten*[1], *Anders Perner*[2], *Anja Boisen*[1]**

[1]*Department of Health Technology, Technical University of Denmark, Kgs. Lyngby, Denmark*
[2]*Department of Clinical Medicine, University of Copenhagen, Copenhagen, Denmark*

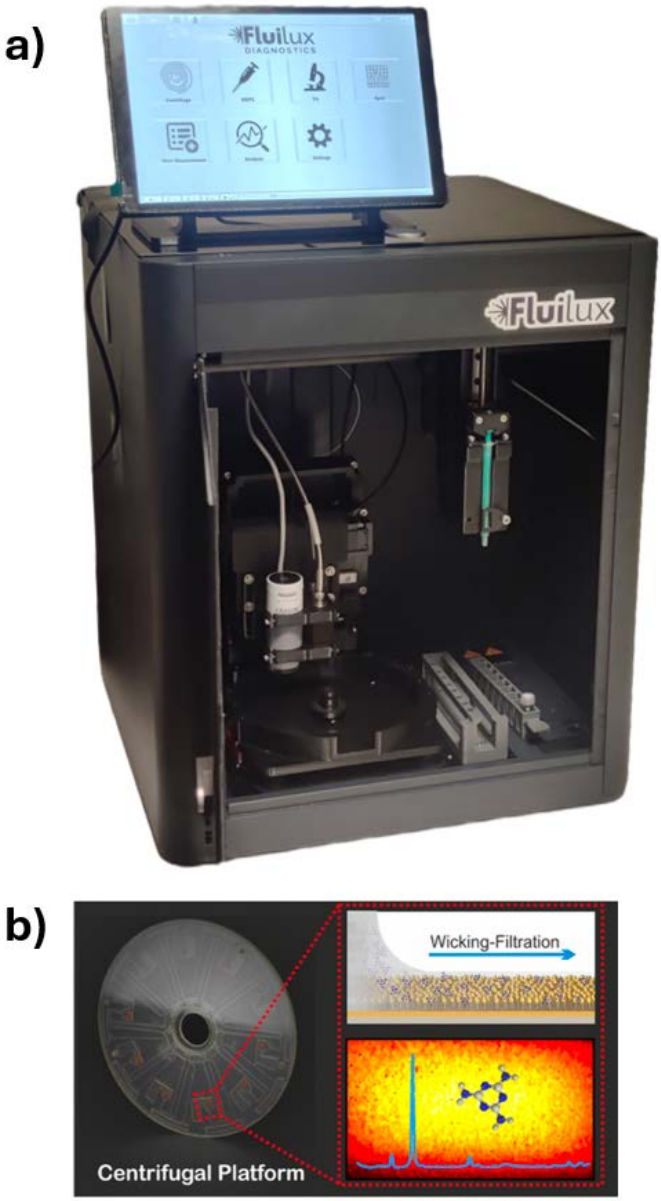
Therapeutic drug monitoring (TDM) of antibiotics in critically ill patients is essential for optimizing dosing, yet current methods rely on bulky chromatographic or immunoassay systems requiring hours to days. No immunoassay kits exist for beta-lactam antibiotics such as meropenem. We present a compact, tabletop hybrid platform combining centrifugal microfluidics with an automated pipetting robot for surface-enhanced Raman scattering (SERS)-based TDM at the point of need.

The two-stage architecture is designed for rapid adaptation to new analytes. Whole blood is loaded onto a centrifugal microfluidic disc for plasma separation and optional ultrafiltration of the free analyte fraction. An automated pipetting robot with a single syringe and access to up to ten solvents then performs advanced sample cleanup, supporting solid-phase extraction (SPE), microextraction by packed sorbent (MEPS), molecularly imprinted polymer (MIP) extraction, dispersive liquid-liquid microextraction (DLLME), and salting-out assisted liquid-liquid extraction (SALLE). New drug targets are addressed by modifying only the solvent protocol, without any cartridge redesign. The purified eluate is returned to the disc, where it contacts silver or gold nanopillar SERS substrates. Nanopillar-assisted separation (NPAS) provides chromatographic-like filtering on the sensor surface, and full-chip Raman mapping is performed by the integrated spectrometer.

Advanced data analysis — partial least squares regression (PLSR), discriminant analysis (PLS-DA), support vector machines (SVM), and one-dimensional convolutional neural networks (1D-CNN) — is applied to SERS mapping data for quantification and discrimination of structurally similar compounds. We demonstrated 100% sensitivity and specificity in discriminating methotrexate from its metabolites (7-OH-MTX, DAMPA) in patient serum, overcoming immunoassay cross-reactivity [Biosens. Bioelectron.: X 2023, 14, 100382]. For meropenem in ICU sepsis management, the platform achieved a detection limit of 12.0 μM and was validated against HPLC with 27 ICU patient samples ($R^2 = 0.8$, $p < 0.05$) [Anal. Chem. 2025, 97, 7888–7896]. Results are obtained within 25–40 minutes, with eight samples processed simultaneously. Because extraction protocols are adapted in software while the consumable disc remains unchanged, new assays can be developed and deployed in weeks rather than months. This positions the platform for expansion beyond antibiotics into antiepileptics, immunosuppressants, and toxicology screening.

Keywords: SERS, therapeutic drug monitoring, centrifugal microfluidics, chemometrics, point-of-need

Figure 1



a) tabletop analyzer with integrated centrifuge, automatic pipetting robot and scanning Raman microscope b) centrifugal microfluidic platform

Posters

[Abstract:0250] [Materials]

Using In Situ Raman Spectroelectrochemistry to Unveil Active-Species Formation During the Oxygen Evolution Reaction on Doped Nickel Oxide

***Jan Ocepek*[1], *Mejrema Nuhanović*[1], *Romana Cerc Korošec*[2], *Marjan Bele*[1], *Nejc Hodnik*[1], *Angelja Kjara Surca*[1]**

[1]*Department of Materials Chemistry, National Institute of Chemistry, Hajdrihova 19, 1000 Ljubljana, Slovenia*
[2]*University of Ljubljana, Faculty of Chemistry and Chemical Technology, Večna pot 113, 1000 Ljubljana*

The growing reliance on fossil fuels and the associated emissions continue to harm the environment, accelerate climate change, and threaten human health. Owing to its high energy density and environmentally benign nature, hydrogen has emerged as a promising alternative to fossil fuels as an energy carrier. Water electrolysis represents an electrochemical route for carbon-free hydrogen production, during which hydrogen is generated at the cathode, while oxygen is obtained during the oxygen evolution reaction (OER) at the anode.

Nickel is a promising catalyst for the OER reaction due to its high activity, stability in alkaline electrolytes, and low cost. Its properties are highly dependent on the presence of dopants, which can improve or hinder the catalytic performance of the catalyst. In our study, we doped nickel oxide with lanthanum. La doping increased OER activity and delayed formation of NiOOH. During electrochemical cycling, however, overpotential required for oxygen evolution of the undoped sample decreased more than for undoped samples. Electrochemical measurements suggest that lanthanum suppresses the oxidation of Ni^{2+} to Ni^{3+}.

We used in situ Raman spectroscopy to follow the formation of active NiOOH species: catalyst ink was drop-casted on roughened gold screen-printed electrode. The peak at ~500 cm^{-1} is attributed to the stretching Ni–O mode of NiO. The pronounced broadness of this band reflects hydroxylation of the powdered samples in the alkaline electrolyte. The band position remains unchanged at the initial potential steps. However, at 0.3 or 0.4 V (vs. Ag pseudoelectrode), two characteristic bands of bending and stretching modes of Ni^{3+}–O state emerge at 482 and 556 cm^{-1}. These peaks are characteristic of γ-NiOOH. These two bands are stronger in intensity, due to resonance Raman enhancement effect. Doping NiO with La3+ shifts this transition to higher potential. During OER, active oxygen species are also observed as a series of low-intensity peaks at 800–1000 cm^{-1}.

Additionally, we used in situ UV-Vis spectroelectrochemistry of a thin-film catalyst deposited on FTO electrodes to follow oxidation state of Ni, which again confirmed a delayed oxidation of nickel in the presence of lanthanum.

Keywords: in situ Raman spectroelectrochemistry, in situ UV-Vis spectroelectrochemistry, oxygen evolution reaction, nickel oxide

[Abstract:0256] [Materials]

Interlayer Optical Phonons in Two-Dimensional Moiré Heterostructures

***Daekwon Lee*[1], *Krishna P Dhakal*[2], *Trang Thu Tran*[2], *Jeongyong Kim*[2], *Heesuk Rho*[1]**

[1]*Department of Physics, Research Institute for Materials and Energy Sciences, Jeonbuk National University, Jeonju, Republic of Korea*
[2]*Department of Energy Science, Sungkyunkwan University, Suwon, Republic of Korea*

Twist-controlled van der Waals heterostructures provide an effective approach for tuning interlayer interactions between atomically thin layers. However, quantifying how twist angle modifies interlayer phonons remains challenging, particularly in crystals with strong in-plane anisotropy. Rhenium dichalcogenides, characterized by a pronounced preferred axis defined by Re atomic chains, offer a useful platform for investigating how the twist angle between two layers influences Raman responses. In this work, we employ Raman spectroscopy, including polarization-resolved measurements, to probe interlayer coupling in twisted $ReS_2/ReSe_2$ heterobilayers. The samples were fabricated by stacking a ReS_2 monolayer on top of a $ReSe_2$ monolayer while intentionally misaligning their Re-chain directions to introduce a controlled twist angle. Low-wavenumber Raman measurements reveal a robust layer-breathing (LB) mode over a wide range of twist angles, whereas no discernible interlayer shear mode is detected within our signal-to-noise limit. Interestingly, the LB peak exhibits a systematic dependence on the twist angle. This behavior suggests that vertical interlayer interactions vary with twist angle due to changes in the relative alignment of atoms at the interface. To quantify the interlayer coupling, we use the LB-mode wavenumbers to extract interlayer force constants using a linear-chain model. The extracted force constants exhibit the same qualitative twist-angle dependence as the LB mode, confirming that interlayer coupling can be tuned by twist. Angle-resolved polarized Raman measurements further enable crystallographic axis identification, ensuring that the twist dependence is evaluated with respect to well-defined Re-chain reference directions. Overall, our results demonstrate a Raman-based approach for controlling and quantifying interlayer interactions in twisted 2D heterostructures, with potential implications for optical and optoelectronic device design.

[This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (Grant No. RS-2025-23324133) and the G-LAMP Program of the NRF grant funded by the Ministry of Education (Grant No. RS-2024-00443714).]

Keywords: Two-dimensional rhenium dichalcogenides, Twisted heterobilayer, Low-wavenumber Raman spectroscopy, Layer breathing mode

[Abstract:0257] [Materials]

Analysis of Solid Polymer Electrolytes Using PHBHx

***Siwoo Kim*[1], *Sujin Lee*[1], *Yeonju Park*[2], *Isao Noda*[3], *Young Mee Jung*[2]**

[1]*Department of Chemistry, Institute for Molecular Science and Fusion Technology, Kangwon National University, Chuncheon 24341, Korea*
[2]*Department of Chemistry, Institute for Molecular Science and Fusion Technology, Kangwon National University, Chuncheon 24341, Korea, Kangwon Radiation Convergence Research Support Center, Kangwon National University, Chuncheon 24341, Korea*
[3]*Department of Materials Science and Engineering, University of Delaware, Newark, DE 19716, USA, Danimer Scientific, Bainbridge, GA 39817, USA*

The rapid growth of the electric vehicle market has significantly increased the demand for high-performance batteries. Consequently, there is a growing a need for next-generation battery systems that not only deliver improved performance but also minimize environmental pollution from battery waste. In addition, to address the safety concerns associated with conventional lithium-ion batteries employing liquid electrolytes, considerable research efforts have been directed toward the development of solid-state electrolytes.

In this study, biodegradable solid polymer electrolytes (SPEs) were prepared through the photopolymerization of poly(ethylene glycol) diacrylate (PEGDA) with the biodegradable polymer poly(hydroxybutyrate-*co*-hydroxyhexanoate) (PHBHx). Its structural and electrochemical properties of the resulting materials were systematically investigated using infrared (IR) spectroscopy, Raman spectroscopy, and electrochemical impedance spectroscopy (EIS). The detailed results and their implications will be presented and discussed.

Keywords: biodegradable polymer, FT-IR spectroscopy, Solid polymer electrolyte

[Abstract:0280] [SERS/TERS/Plasmonics]

A Magnet-integrated Paper Chip for On-site Enrichment and SERS Detection of Neglected Tropical Diseases

Mengdan Lu*, *Jaebum Choo

Department of Chemistry, Chung-Ang University, Seoul, South Korea

Surface-enhanced Raman scattering (SERS) is a powerful spectroscopic technique for biosensing due to its molecular fingerprint specificity and high sensitivity. Integrating SERS with paper-based chips enables the development of low-cost, simple, and easy-to-use biosensors. However, a fundamental limitation of paper-based SERS assays arises from the random distribution of SERS nanotags within the porous cellulose fiber network. Since SERS spectra are collected from a micron-scale laser excitation volume, only a limited number of randomly dispersed nanotags are sampled during measurement, resulting in relatively weak SERS signals, particularly at low analyte concentrations. To address this challenge, we developed a magnet-integrated vertical flow paper chip that integrates immunoreaction, magnetic enrichment, and SERS detection within a single paper device. In this platform, 1 μm magnetic beads form sandwich immunocomplexes with target analytes and SERS nanotags. Under an external magnetic field, the magnetic bead-based immunocomplexes rapidly accumulate in a confined detection region on the chip, effectively increasing the local density of SERS nanotags within the laser focal volume. This magnetic enrichment significantly improves SERS signal intensity and reproducibility compared with conventional paper-based assays, where nanotags remain randomly dispersed along paper fibers. Unlike many magnet-assisted microdroplet systems that measure SERS signals from the supernatant and produce inverse responses, the proposed platform directly detects magnetic bead-based immunocomplexes, generating a positive SERS signal correlated with target binding. The proposed platform is being explored for the detection of neglected tropical diseases (NTDs), including Dengue, Zika, Yellow Fever, and Chikungunya. This work demonstrates an effective strategy to improve SERS sampling efficiency on paper-based devices and provides a promising approach for in vitro diagnostics in resource-limited settings.

Keywords: Surface-enhanced Raman scattering (SERS), Magnetic bead enrichment, Paper-based biosensor, Neglected tropical diseases

[Abstract:0281] [SERS/TERS/Plasmonics]

A Molecularly Imprinted SERS Sensor for Label-free Quantitation Whole Exosomes in Biofluids

Jiadong Chen*, *Jaebum Choo

Department of Chemistry, Chung-Ang University, Seoul, South Korea

Sensitive and reliable exosome detection as cancer biomarkers remains challenging due to low abundance and the coexistence of interference species in biofluids. Here, by integrating a molecularly imprinted polymer (MIP) recognition layer into a surface-enhanced Raman scattering (SERS) substrate, we develop a highly sensitive and selective label-free exosome assay in biological samples without any sample preparation. The MIP–SERS platform was constructed by the immobilization of exosome templates onto a nano-popcorn SERS-active substrate using 4-mercaptophenylboronic acid (4-MPBA), through reversible covalent bonds between the glycoproteins on the exosomal surface and the boronate group. Next, a polydopamine (PDA) nanocoating with controllable thickness and density was generated on the substrate via spontaneous dopamine self-oxidation. After exosome removal, high-affinity nanocavities with shape complementarity and tailored surface chemistry were obtained. The label-free detection mechanism consists of the following simple steps: First, the target exosomes are selectively recaptured through the synergistic contributions of noncovalent interactions between PDA and exosomal functional groups, shape selectivity of the imprinted cavities, and boronate interaction between 4-MPBA ligands and glycan groups of the exosome. Next, quantification of exosomes was performed through a blocking mechanism by immersing the platform into the IR-792 Raman reporter: in the absence of exosomes, Raman reporter molecules readily access the plasmonic gold surface, providing an intense SERS signal; once exosomes specifically occupy the imprinted nanocavities, IR-792 diffusion to the substrate is blocked, leading to quenching of the SERS signal. This platform enables rapid and highly sensitive exosome detection in complex biological fluids, highlighting its promise for point-of-care cancer diagnostics.

Keywords: Surface-enhanced Raman scattering (SERS), Molecularly imprinted polymer (MIP), Exosome, Label-free exosome assay

[Abstract:0288] [SERS/TERS/Plasmonics]

Alginate-based Hydrogel Composites for Surface-Enhanced Raman Spectroscopy Applications

***Barbora Štefková*, Robert Prucek**

Department of Physical chemistry, Faculty of Science, Palacký University Olomouc, 17. Listopadu 12, 771 46, Olomouc, Czech Republic

The exploration of hydrogel-based substrates for surface-enhanced Raman spectroscopy (SERS) has increased significantly in the past five years due to their versatility and several advantages compared to conventional SERS substrates, such as colloidal nanoparticle suspensions or metal nanoparticle layers deposited on solid supports. Hydrogels provide an optically transparent environment with minimal intrinsic spectral background, which is advantageous for SERS analysis. In addition, their flexible and highly hydrophilic nature, resulting from strong hydrogen bonding and water-binding capacity, helps to overcome the "coffee-ring" effect commonly observed during analyte deposition on solid substrates. Hydrogels may also enhance nanoparticle stability; in particular, sodium alginate offers favorable stabilization properties. As mentioned alginate hydrogels are the focus of the presented ongoing study.

This work investigates the preparation of Ag–alginate hydrogel composites and their application as SERS substrates. Ag-Alginate hydrogel composites were prepared using various reducing agents for Ag+ reduction (trisodium citrate, ascorbic acid and others) and different concentration of sodium alginate (1-5% w/w). Calcium ions (Ca^{2+}) were employed as cross-linking agents to form the hydrogel network. The prepared substrates were characterized using UV–Vis spectroscopy, Raman spectroscopy, Fourier-transform infrared spectroscopy (FTIR), and scanning electron microscopy (SEM).

The SERS activity of the prepared hydrogel substrates was evaluated using excitation wavelengths of 455, 633, and 785 nm. Several common Raman reporter molecules were used as analytes, including rhodamine B, rhodamine 6G, crystal violet, and adenine. Analytical enhancement factors were calculated and the limits of detection for each system were determined. Reproducibility of the SERS response was assessed by calculating the relative standard deviation (RSD) from measurements collected at ten different points on each substrate. In addition, substrate stability was investigated by comparing samples stored under hydrated conditions with those stored in a dried state and were subsequently rehydrated in analyte solution prior to analysis.

Keywords: Surface-enhanced Raman spectroscopy, Alginate hydrogels, Silver nanoparticles

Posters

[Abstract:0292] [Theory/Computation]

Structural and Vibrational Characterisation of Human Milk Oligosaccharides by Raman, Raman Optical Activity, and DFT Vibrational Calculations

***Heber Islas Rios*[1], *Jeremy D Landry*[2], *Jessica Holien*[1], *Paul A Ramsland*[1], *Ewan W Blanch*[2]**

[1]*Department of Biology, RMIT University, Victoria, Australia*
[2]*Department of Applied Chemistry and Environment Sciences, RMIT University, Victoria, Australia*

Glycans play an essential role in biological systems by participating in several processes related to energy source and storage, serve as structural components, have a role in cell signaling, immune response, and movement. Although the importance of glycans in biological processes has recently been highlighted, their structural characterisation and detailed understanding of their interactions with other biomolecules remain challenging due to their conformational flexibility and stereochemical diversity. A particularly important class of glycans is human milk oligosaccharides (HMOs), which are highly abundant in human milk and fulfil critical biological functions, including the prevention of pathogen adhesion, the modulation of immune responses, and the promotion of infant gut development. Within this group, 2'-Fucosyllactose (2'-FL) and 3'-Fucosyllactose (3'-FL) are the most prevalent oligosaccharides in HMO. These components are not digested and reach the colon, where they undergo partial fermentation, acting as a soluble prebiotic fibre. To analyse and characterise 2'-FL and 3'-FL, we employed molecular dynamics and DFT calculations to predict the structural and vibrational properties, beginning with their individual component saccharides: glucose, galactose, and fucose, lactose, as well as the complete molecules 2'-FL and 3'-FL. Computational spectral predictions, both individual and global, were compared with the experimental spectra to determine which bands arise from contributions of each monosaccharide or from a combined or synergistic effect. These findings demonstrate that vibrational spectroscopic techniques, both computational and experimental, provide a powerful approach for the characterisation of glycans, as illustrated here for the HMOs 2'-fucosyllactose and 3'-fucosyllactose.

Keywords: Glycans, Human Milk Oligosaccharides, DFT, Raman Optical Activity

[Abstract:0294] [SERS/TERS/Plasmonics]

Formation of Ag core–Au shell Nanostructures with Surface-reduction

***Yeseul Park*[1], *Dae Hong Jeong*[2]**

[1]*Department of Chemistry Education, College of Education, Seoul National University, Seoul, Republic of Korea*
[2]*Department of Chemistry Education, College of Education, Seoul National University, Seoul, Republic of Korea, Learning Science Research Institute, Seoul National University, Seoul, Republic of Korea*

Ag core–Au shell nanostructures are attractive because they combine the strong plasmonic response of Ag with the chemical stability of Au. However, conventional Au shell growth often requires separate reducing and growth-directing agents, and undesired bulk reduction or homogeneous nucleation can interfere with controlled shell formation. Here, we propose a surface-selective synthetic strategy for Ag core–Au shell nanostructures driven by the cooperative functions of interfacially pre-positioned 4-aminothiophenol (4-ATP) and poly(vinylpyrrolidone) (PVP). In this system, 4-ATP is introduced between the Ag core and Au shell and serves not merely as an interfacial spacer, but as an active interfacial molecule that directly contributes to Au precursor reduction and promotes shell deposition on the existing Ag surface. As a result, Au growth proceeds preferentially at the Ag surface rather than through random reduction in the bulk solution. In addition, 4-ATP functions as a Raman internal standard, thereby providing both structural and spectroscopic utility within the same nanostructure. PVP, while primarily acting as a colloidal stabilizer, also assists the reduction of Au species and supports interfacial shell growth in cooperation with 4-ATP. These results indicate that the present reaction does not proceed through bulk-phase reduction, but through an interface-directed growth mechanism in which a pre-positioned functional molecule and a stabilizing polymer cooperatively induce shell deposition. This strategy highlights how multifunctional interfacial molecules can precisely regulate both the spatial location and reaction pathway of shell growth without the use of an additional reductant. The present approach provides a new synthetic concept for the controlled formation of Ag–Au core–shell nanostructures and suggests a versatile platform in which interfacial molecular design is directly coupled to both nanoscale growth control and Raman functionality.

Keywords: Surface-reduction, core-shell nanostructure, Interfacial 4-Aminothiophenol

[Abstract:0295] [Coherent Raman Imaging]

Label-Free Sub-Micron Imaging of Cellulose Microfibrils in *Pseudotsuga menziesii* by Multimodal SHG and CARS Microscopy

***Ting Hao Chen*[1], *Guy Costa*[2], *Philippe Leproux*[3], *Ryo Suzuki*[1], *Hideaki Kano*[1]**

[1]*Faculty of Science and Technology, Keio University, Yokohama, Japan*
[2]*LABCiS, Faculté des Sciences et Techniques, Université de Limoges, Limoges, France*
[3]*Institut de Recherche XLIM, UMR CNRS 7252, Université de Limoges, Limoges, France*

Cellulose is among the most abundant biopolymers in nature and a primary structural component of plant cell walls. In these walls, cellulose is organized into bundled structures known as cellulose microfibrils (CMFs), which play a decisive role in determining the mechanical properties and growth anisotropy of plant tissues [Biomacromolecules, 2023, 24, 4759-4770]. While cellulose is also widely recognized as a vital renewable resource for biofuels such as bioethanol, its functional role and industrial utility are fundamentally governed by the architecture of these CMFs. However, the exact spatial distribution, structural organization, and functional role of CMFs within the cell wall remain only partially understood, largely due to the challenge of directly visualizing them at sub-micron scales without labeling.

In this study, we employed second-harmonic generation (SHG) and coherent anti-Stokes Raman scattering (CARS) microscopy [Anal. Chem. 2025, 97, 28, 15299-15309] to investigate the distribution and molecular characteristics of CMFs in Douglas-fir (Pseudotsuga menziesii) wood. SHG imaging revealed distinct signal domains within the cell wall, while CARS spectroscopy provided molecular information on cellulose, lignin, and other cell wall components (Fig.1).

The SHG signal appeared as non-continuous domains in the cell wall and exhibited strong polarization dependence, suggesting the presence of highly ordered crystalline structures with specific orientations. Based on these characteristics, the observed SHG signals are likely to reflect the organized structure of CMFs. Polarization-dependent SHG analysis further indicated that CMFs are preferentially aligned along the boundary between adjacent cell walls, and the principal axis of the nonlinear optical response closely corresponds to the orientation of the cell wall interface (Fig.2).

These results demonstrate that multimodal SHG and CARS microscopy provides a powerful label-free approach for visualizing CMF organization and chemical heterogeneity in wood at the sub-micron scale. Our findings suggest that CMF orientation is closely associated with cell wall architecture and may contribute to the regulation of cell shape and growth anisotropy in wood tissues.

Keywords: CARS, SHG, Cellulose Microfibril, Polarization, Microscopy

Figure 1. CARS and SHG images showing the distribution of molecular and crystalline components in the cell walls of *Pseudotsuga menziesii*.

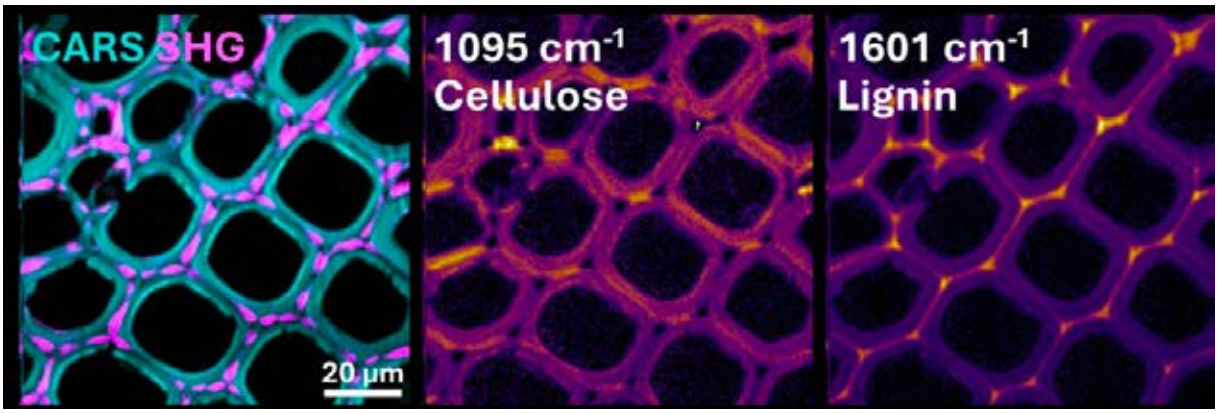
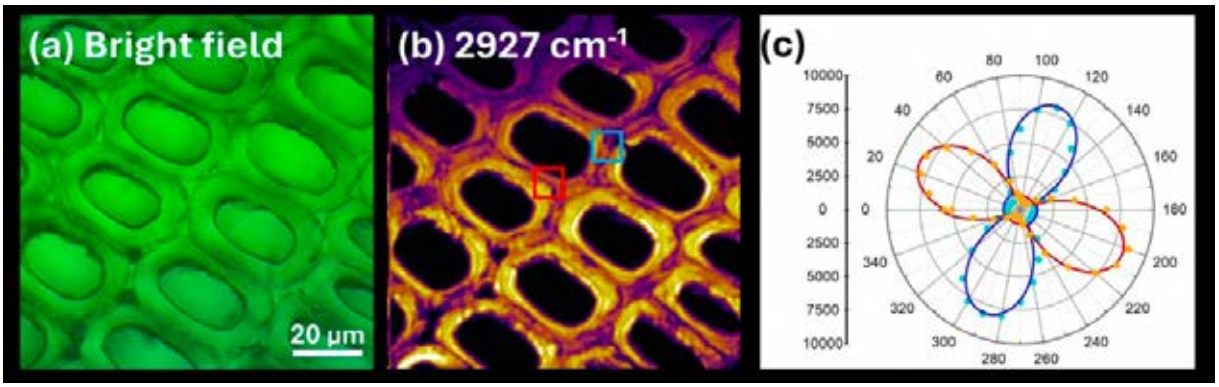


Figure 2. (a) Brightfield and (b) CARS images showing the cell wall morphology. (c) Polar plot of the SHG intensity as a function of incident laser polarization angle, recorded at the position indicated in (b). The data reflects the local orientation



[Abstract:0296] [SERS/TERS/Plasmonics]

Design and Evaluation of Gold-Based Plasmonic Platforms for SERS Detection in Complex Biological Systems

***Dragos Ioan Olariu*[1], *Septila Renata*[2], *Ciprian Paul Mairean*[2], *Valentin Toma*[3], *Magdalena Aflori*[4], *Brindusa Dragoi*[5], *Rares Stiufiuc*[6]**

[1]*Nanotechnology Laboratory, TRANSCEND Research Center, Regional Institute of Oncology, Iasi, Romania; "Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania*
[2]*Nanotechnology Laboratory, TRANSCEND Research Center, Regional Institute of Oncology, Iasi, Romania*
[3]*Department of NanoSciences, Institute of Biomedical Research - MedFUTURE, "Iuliu Hatieganu" University of Medicine and Pharmacy, Cluj Napoca, Romania*
[4]*"Petru Poni" Institute of Macromolecular Chemistry, Iasi, Romania*
[5]*Nanotechnology Laboratory, TRANSCEND Research Center, Regional Institute of Oncology, Iasi, Romania; Faculty of Chemistry, "Alexandru Ioan Cuza" University of Iasi, Iasi, Romania*
[6]*Nanotechnology Laboratory, TRANSCEND Research Center, Regional Institute of Oncology, Iasi, Romania; Department of NanoSciences, Institute of Biomedical Research - MedFUTURE, "Iuliu Hatieganu" University of Medicine and Pharmacy, Cluj Napoca, Romania*

Surface-enhanced Raman spectroscopy (SERS) has emerged as a powerful analytical technique for ultrasensitive molecular detection due to its ability to amplify Raman signals through localized surface plasmon resonance (LSPR) phenomena. The efficiency of SERS detection is strongly governed by the physicochemical characteristics of the plasmonic substrates, including nanoparticle morphology, surface chemistry, and interparticle coupling that promotes electromagnetic hotspot generation.

In this study, engineered gold nanostructures were developed as plasmonic platforms aimed at improving Raman signal enhancement and spectral reproducibility. Gold nanoparticles synthesized through seed-mediated growth were employed to obtain controlled nanoscale architectures capable of supporting efficient plasmonic coupling. Surface functionalization strategies were implemented in order to tailor nanoparticle–analyte interactions and to improve colloidal stability under conditions relevant for spectroscopic measurements.

The performance of the fabricated substrates was systematically evaluated using well-established Raman probe molecules such as methylene blue (MB) and rhodamine 6G (R6G). Spectral measurements were conducted under both 633 nm and 785 nm laser excitation to examine the influence of excitation wavelength and nanoparticle surface environment on signal amplification. Comparative analysis between citrate-stabilized nanospheres and anisotropic CTAB-directed nanostructures enabled the investigation of morphology-dependent enhancement mechanisms.

Furthermore, key experimental parameters including nanoparticle size distribution, surface charge characteristics, and aggregation control were correlated with the stability and reproducibility of the SERS response. These aspects are critical for developing reliable plasmonic sensing platforms suitable for analytical and biomedical applications.

To assess the applicability of the developed substrates in biologically relevant environments, preliminary label-free SERS measurements were performed on human serum samples obtained from patients diagnosed with pancreatic and gastric cancer, together with control samples from healthy donors. The resulting spectra reveal the complex biochemical signatures present in serum and demonstrate the potential of engineered plasmonic nanostructures to capture disease-associated molecular fingerprints within heterogeneous biological matrices.

Keywords: Surface-Enhanced Raman Spectroscopy, Gold Nanoparticles, Plasmonic Substrates, Biomedical Sensing, Serum Analysis

[Abstract:0297] [SERS/TERS/Plasmonics]

SERS Probing of Biomolecular Interactions of Gold Nanoparticles during Cellular Processing in Co-Cultures

***Anastasiia Kniazeva*, Cecilia Spedalieri, Janina Kneipp**

Department of Chemistry, Humboldt University of Berlin, Berlin, Germany

The interaction between nanoparticles and intracellular biomolecules is important for developing and optimizing nanoparticle-based systems used in targeted drug delivery, optical probing and various diagnostic and bioanalytical applications. While single cell lines are widely used to study intercellular processes, they fail to capture the intercellular interactions and biochemical complexity present in tissues and organs. Understanding how the protein corona formed in one cellular environment affects processing in another is therefore essential for understanding biomolecule interaction in complex biological systems. Surface-enhanced Raman scattering (SERS) is a powerful analytical tool for this purpose because it allows to probe and detect molecules or functional groups that are in the vicinity of metal nanoparticle.

In this study, two types of mammalian cell lines were used to study how cellular processing of citrate stabilized gold nanoparticles by one cell type affects the interactions and distribution inside cells of another cell type. The chemical composition of the biomolecules interacting with the nanoparticles was probed using SERS under different incubation regimes and co-culture conditions.

Keywords: Surface-enhanced Raman scattering (SERS), Cell co-cultures, Biomolecule–nanoparticle interactions

[Abstract:0299] [Biology/Biomedicine]

Crystalline Guanine Formation in Microalgae: Study of Preferred Nitrogen Sources Using Isotopic Labelling and Raman Microscopy

***Alexandra Suchá*, Peter Mojzes**

Institute of Physics, Faculty of Mathematics and Physics, Charles Universty, Prague, Czech Republic

The recent discovery that unicellular eukaryotes from all major supergroups can accumulate nitrogen reserves in the form of crystalline purines, preferentially guanine, has prompted a detailed investigation of the molecular mechanisms underlying these processes. The formation of intracellular crystals and the subsequent utilization of stored nitrogen for growth have been studied in the greatest detail in the marine dinoflagellate *Amphidinium carterae*. In this model organism, a close relative of the endosymbiotic zooxanthellae of corals, it was found that, in addition to *de novo* biosynthesis from simple nitrogen-containing precursors (nitrate, ammonium, urea), *A. carterae* can quickly and efficiently accumulate some purines directly from the environment and store them in crystalline form. This ability is not limited to purines; as recently shown, *A. carterae* can also transport and crystallize pyrimidines and pterins [Nat. Biotechnol. 2026]. The direct and rapid accumulation of various N-heterocycles assumes the involvement of a robust constitutive transport mechanism. For *A. carterae*, it appears to be a preferred route over *de novo* biosynthesis. Since crystalline purines have been observed in a wide range of unicellular eukaryotes, the question arises whether this preference is a general feature or whether other eukaryotes, although living in the same environment, can exhibit different preferences.

Here, we compare direct guanine transport and *de novo* biosynthesis in *Chromera velia*, an apicomplexan photoparasitic marine microalga infecting coral larvae. Nitrogen-starved *C. velia* were grown in media simulating a marine environment enriched with dissolved guanine in combination with another nitrogen source (nitrate, ammonium, urea). Subsequently, the formation of crystalline guanine was detected directly in intact cells using Raman microscopy. To distinguish the sources of crystalline guanine, isotopically labelled precursors containing ^{15}N were used. Thanks to the sensitivity of Raman spectra to isotopic substitution, it was possible to trace the origin of nitrogen in the accumulated guanine. At the same time, nitrogen source utilization for culture growth was monitored. It was found that, unlike *A. carterae*, *C. velia* probably lacks an efficient constitutive mechanism for direct transport of guanine and prefers *de novo* biosynthesis of crystalline guanine from nitrate.

This work was supported by Charles University (SVV-2025-260832).

Keywords: Chromera velia, guanine crystals, de novo biosynthesis, direct uptake, Raman microscopy

[Abstract:0300] [Materials]

Recent Advances in Stable Electrodes for Two-Dimensional Materials Guided by Raman Spectroscopy

Kulurumotlakatla Dasha Kumar

College of Energy, College of Chemistry and Chemical Engineering, State Key Laboratory of Physical Chemistry of Solid Surfaces, The MOE Key Laboratory of Spectrochemical Analysis and Instrumentation, College of Materials, Xiamen University, Xiamen 361005, China.

Ever since they were discovered, transition-metal carbides Mxene, especially Ti3C2Tx have become a cornerstone of advanced electrochemical research. Unlike many 2D materials, Mxenes combine clay-like processability with metallic conductivity. In practice, though, they face two big hurdles: irreversible nanosheet restacking and surface oxidation/unstable terminations (-OH, -O, -F) can lead to parasitic reactions, further degrading the long-term cycle life of the electrode. Raman spectroscopy offers a non-destructive way to tackle these issues. By tracking phase purity and defect density, it helps diagnose Mxene electrodes in real time. In this work, we show that a modification in electrochemical changes to surface terminations alter the Raman response, and we expand a Raman-spectra library for the most common Mxenes. Monitoring the A1g (Ti, O, C) and Eg modes between 100–800 cm-1 reveals the lattice breathing peak shifts and broadening that map to ion intercalation and strain. For carbon-integrated Mxene hybrids, the (ID/IG) intensity ratio gives a direct metric of sp2 integrity. Ultimately, Raman analysis correlates molecular-level vibrations with macro-scale performance, providing an agenda for engineering the next generation of stable, high-capacity energy storage devices.

Keywords: Raman spectroscopy, SERS, Mxene, material characterization, two-dimensional materials

Posters

[Abstract:0301] [SERS/TERS/Plasmonics]

Magnetic Polystyrene Beads Coated with Au and Ag Nanoparticles for SERS Detection of Staphylococcus Aureus Infection and an Alzheimer's Disease Biomarker

***Robert Prucek*[1], *Barbora Štefková*[1], *Milan Kolář*[2], *Jiří Gallo*[3]**

[1]*Department of Physical Chemistry, Faculty of Science, Palacký University in Olomouc, 17 Listopadu 12, 771 46, Olomouc, Czech Republic*
[2]*Department of Microbiology, Faculty of Medicine and Dentistry, Palacký University Olomouc, Hněvotínská 3, 775 15, Olomouc, Czech Republic*
[3]*Department of Orthopaedics, Faculty of Medicine and Dentistry, Palacký University Olomouc, I. P. Pavlova 6, 77520, Olomouc, Czech Republic*

Effective and targeted disease treatment requires rapid and reliable identification of specific biomarkers. Surface-enhanced Raman spectroscopy (SERS), when combined with the streptavidin–biotin interaction, represents a promising alternative to conventional detection techniques such as culture-based assays or PCR. Because a wide variety of biotinylated antibodies are commercially available, this approach provides a versatile platform for numerous analytical applications.

In this work, we introduce a rapid and straightforward method for the preparation of streptavidin-coated magnetic polystyrene–Au (or Ag) nanocomposite particles that serve as efficient substrates for SERS analysis. Commercially available streptavidin-modified polystyrene (PS) microparticles containing a magnetic core were used as the starting material for the fabrication of SERS-active and magnetically separable composites. Gold or silver nanoparticles were deposited onto these particles through the reduction of Au(III) or Ag(I) ions using either ascorbic acid or dopamine as reducing agents. The selected reducing agent significantly affects the morphology and size of the resulting Au or Ag nanoparticles, which ranged from 15 to 100 nm.

The prepared composites were characterized using transmission electron microscopy, elemental mapping, and magnetization measurements. The amounts of gold and silver were quantified by atomic absorption spectroscopy (AAS). Compared with magnetic composites based on iron oxides, the synthesized materials exhibit substantially lower density, which reduces their tendency to sediment. In addition, the presence of a polystyrene shell surrounding the magnetic iron oxide core markedly limits particle aggregation. Notably, the preparation and purification of this SERS substrate can be completed within only a few minutes.

Finally, the PS composites decorated with thorn-like Au nanoparticles (~ 100 nm) were successfully applied for the specific and selective detection of Staphylococcus aureus infection in knee joint fluid associated with prosthetic joint infection (PJI), as well as for the detection of tau protein, a biomarker related to Alzheimer's disease.

Keywords: SERS, Magnetic nanocomposites, AgNPs, AuNPs, Biosensing, Streptavidin–biotin interaction

[Abstract:0308] [Industrial/Societal Applications]

Aquatic Aged Micro- Nano Plastic Reference Materials as Resonance Raman-SERRS Traceable Probe for Controlled Exposure and Impact Studies

***Simona Pinzaru*[1], Ion Nesterovschi[1], Ioana Cârdan[1], Karlo Maškarić[1], Anamaria Couți[1], Csilla Molnar[2], Geza Lazar[1], Lucian Barbu Tudoran[3], Maria Suciu[3], Tudor Tămaş[4], Branko Glamuzina[5], Vera Slaveykova[6]**

[1]*Biomolecular Physics Department, Babeş–Bolyai University, Kogălniceanu 1, RO-400084, Cluj-Napoca, Romania*
[2]*Institute for Research, Development and Innovation in Applied Natural Sciences, Babes-Bolyai University, Fântânele 30, RO-400327 Cluj-Napoca, Romania*
[3]*National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, 400293, Romania*
[4]*Faculty of Biology and Geology, Babes-Bolyai University, Kogalniceanu 1, 400084 Cluj-Napoca, Romania*
[5]*Department of Applied Ecology, University of Dubrovnik, Ćira Carića 4, 20000 Dubrovnik, Croatia*
[6]*Department F.A. Forel for Environmental and Aquatic Sciences, Faculty of Sciences, University of Geneva, 66 Boulevard Carl-Vogt, 1211 Genève 4, Switzerland*

Current efforts in advancing nano plastics research depend on reference materials, relevant and comparable to those found in environmental or food samples. However, microplastics co-exist with nano plastics in real-world samples. Their natural distribution, quantification and control cannot be addressed simultaneously, as techniques and methodologies for microplastics are advanced and Raman techniques leads this advancement, while nano plastics detection and quantification are yet facing challenges. The existent certified reference nano plastics increasingly available commercially in the last few years provide several micro- or nano plastics species as standard, not environmental relevant probes. Cascade filtrations for fraction separation are the protocols widely described and the resulted fractions are handled by different techniques for exposure, intake control, effects and impact studies.

Here, we address this issue from nature-inspired material: we recovered aquatic aged macro plastics environmentally relevant, extensively used in human activity and turned it in relevant, micro-nano plastics powders and suspensions, as lab-certified reference material, highly demanded for advancing studies on plastic toxicity and impact on living organisms and trophic chain transmission to our plate and health.

Seven types of powders and suspensions are obtained and comprehensively characterised using primarily Raman spectroscopy techniques in conjunction with IR, XRD, SEM-EDX and DLS methods. Doing so, we advance our understanding in micro-nano plastics behaviour in aquatic environment, their handling requirements and provide robust, reference material for further advancing toxicology studies while supporting with Raman tools the evidence of plastics intake and detection either at micro- or nano level. We emphasised here the crucial importance of Raman technology involved in this comprehensive process control and benefit from the combination of enhancement techniques to detect and track persistent pigments embedded in micro-nano plastic, when plastic itself provides too weak signal to be traceable. Thus, plastic cycle in nature, fully addressed via Raman technology provides first robust prerequisite to properly address its long-term effects on our waters, food and health.

This research is part of a large innitiative under the IMPACT “Implications of Nano/Microplastic Pollution on AquatiC Environment HealTh” Project financed within the framework of the second Swiss Contribution MAPS,

No. 1Z11Z0_230154 and Nr. 7ROCH /07.2025.

Keywords: aged micro-nano plastics; relevant certified reference material, Raman technology, enhancement techniques, impact

Fig. 1. Example of pigmented plastic recovered from sea bottom and transformed in powdered micro-nanoplastic with controlled size distribution while traceable at submicrometer size level using resonance Raman spectroscopy.

The pigment embedded in nano plastic as a veritable Trojan horse bearing inside a resonance Raman probe which can be tracked using enhancing Raman techniques along the aquatic trophic chain.

[Abstract:0312] [Non-linear/Time-resolved]

A Time-Domain (Raman) Spectroscopy Instrument for Identifying Minerals and Gases in Space Exploration?

***Yookyung Ha*[1], *Emma Kinne*[1], *Sergey G. Pavlov*[2], *Nikola Stojanovic*[2], *Michael Gensch*[1]**

[1]*Institute of Physics and Astronomy, Technische Universität Berlin, Berlin, Germany, Institute of Space Research, German Aerospace Center (DLR), Berlin, Germany*
[2]*Institute of Space Research, German Aerospace Center (DLR), Berlin, Germany*

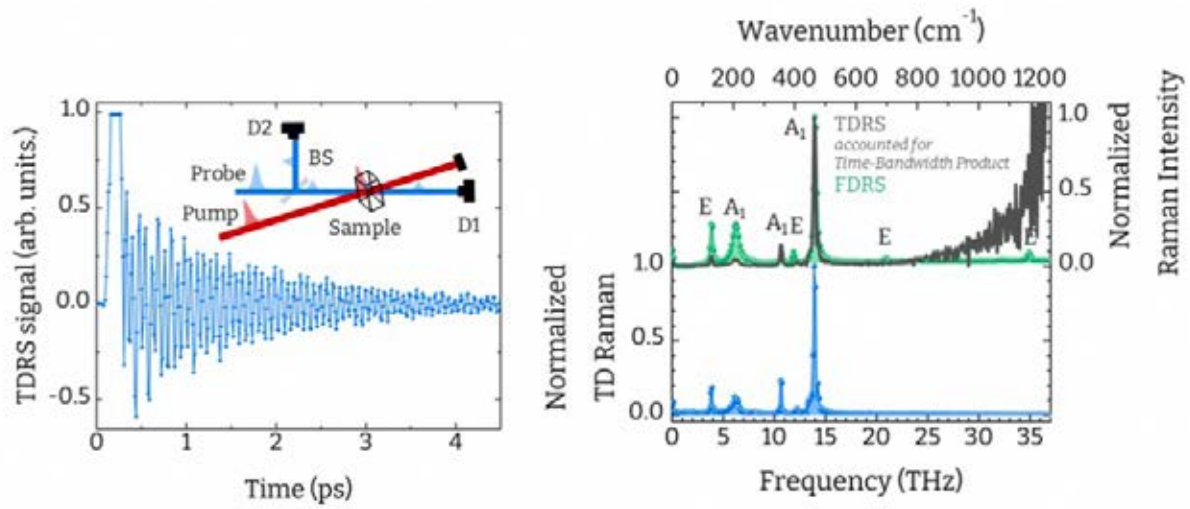
Conventional Raman spectroscopy is an established technique for the identification of materials by their vibrational fingerprint. Therefore, Raman instruments are now frequently considered for incorporation into space exploration missions to celestial bodies of our solar system. With the development of space-qualified femtosecond lasers, the use of time-domain based spectroscopic methods such as Time-domain Raman Spectroscopy (TDRS) and Rotational Coherent Raman Scattering (RCRS) has become a viable alternative. These techniques complement conventional Raman techniques by detecting Raman-active fingerprints while being inherently unaffected by ambient light or photoluminescent background. Moreover, time-domain techniques have a large potential for chip-integration leading to much more compact and robust instruments. Recently, we reported that TDRS is a viable alternative to Raman spectroscopy for identifying space relevant minerals (Figure 1).

In this work, we show that a slight modification of our experimental setup, previously designed to characterize the lattice dynamics of minerals, can also be employed to detect molecular species sensitively via RCRS. When molecules with anisotropic polarizability interact with an intense ultrashort laser pulse, their response manifests as periodic rotational revivals with a periodicity that depends on the molecular constant (Figure 2a,c). As a result, we can identify the rotational revival signatures of N_2 and O_2 in air at 295K and 1 bar. Our results show good agreement with theoretical simulations performed with the LIMAO software (Figure 2c).

Furthermore, simulations show that our setup can measure other linear and symmetric-top molecules under certain extraterrestrial conditions. With this time-domain spectroscopic instrument, not only can one characterize both minerals and gases with a single measurement, but also identify them from the phonon frequencies and molecular-specific periodicities of the revivals. Therefore, this technique shows potential for space exploration, especially in conditions where planetary atmospheres comprise gas molecules such as homonuclear diatomics (N_2, O_2), linear triatomics (CO_2, SO_2), and some hydrocarbons.

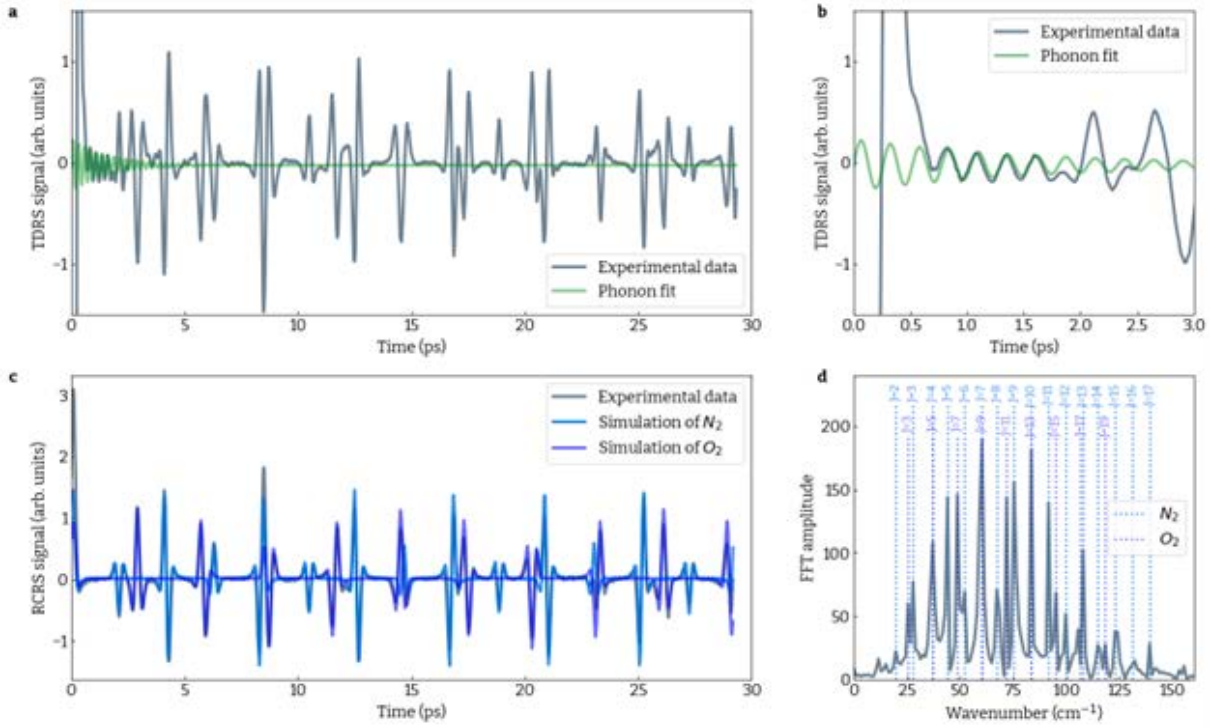
Keywords: Time-domain spectroscopy, gases, minerals, rotational coherent scattering, planetary research

Figure 1



TDRS measurement of transient transmission on α-quartz (Korth Kristalle, Germany) and the detection geometry shown in the inset (left). The Fourier transform of the time-domain signal is shown in the bottom panel and the Frequency-Domain Raman (FDRS) spectrum is also shown in green for comparison (right). Figure adapted from [J. Raman Spectrosc. 2025, 56, 9, 916-919]

Figure 2



(a) Experimental measurement of Time-Domain Raman spectroscopy (TDRS) performed on quartz in air at 295 K and 1 bar fitted with the phonon mode at 3.9 THz of quartz, and (b) its zoomed-in figure. (c) Experimental measurement of Rotational Coherent Raman Scattering (RCRS) in air at 295 K and 1 bar compared to the simulations of rotational dynamics of nitrogen and oxygen. (d) The Fourier Transform spectrum of the RCRS experimental data, where each peak represents the energy transition between the rotational levels J allowed by the Raman selection rules.

Posters

[Abstract:0316] [Biology/Biomedicine]

Influence of Tissue Turbidity on Optimal Raman Offset for Transcutaneous Bone Measurement

***Joseph O'Halloran*, Rosha Murphy, Jakub Byrdziak, Suraj Kumar Kothuri, Pranav Lanka, Sanathana Konugolu Venkata Sekar, Stefan Andersson Engels, Rekha Gautam**

Biophotonics@Tyndall, Tyndall National Institute, Cork, Ireland

Spatially offset Raman spectroscopy (SORS) enables the measurement of samples through highly turbid media, including transcutaneous bone, by varying the source–detector offset to increase the relative contribution of subsurface layers to the measured signal. However, in vivo applications are complicated by variability in the optical properties and geometry of overlying tissues, which influence photon migration and therefore offset selection.

In a recent paper from our group [1], a novel metric, the enhancement-to-noise ratio (ENR), was introduced to calculate the optimal SORS offset for transcutaneous bone measurements. The ENR determines the offset that balances top-layer signal suppression with minimisation of the coefficient of variation of the bottom-layer signal.

Here, to further guide offset selection, we present a systematic evaluation of how superficial tissue optical properties influence ENR-based optimisation in transcutaneous Raman measurements, combining phantom measurements with adjoint Monte Carlo (aMC) modelling.

To mimic the transcutaneous bone geometry experimentally in a controlled manner, we use two-layer phantoms with top layers of various thicknesses and optical properties overlying a bone-mimicking phantom composed of hydroxyapatite (HAP) and ammonium chloride (NH_4Cl). Each layer contains a distinct Raman peak, enabling independent analysis of the top- and bottom-layer signals.

By clarifying how the ENR behaves with top-layer optical properties and thicknesses, this study aims to support more accurate selection of the optimal Raman offset for transcutaneous bone measurements. This represents a step toward noninvasive Raman-based assessment of bone health.

Reference:

[1] Ma, H.; Lanka, P.; Kothuri, S. K.; Jayet, B.; Mahadevan-Jansen, A.; Andersson-Engels, S.; Konugolu Venkata Sekar, S.; Gautam, R. Raman Spectroscopy Based Framework for In-Vivo Assessment of Bone Composition. J. Phys. Photonics 2026, 8 (1), 015065. https://doi.org/10.1088/2515-7647/ae485e.

Acknowledgements:

This work is conducted with the financial support of Taighde Éireann—Research Ireland Professorship (SFI/22/RP-2TF/10293) and Pathway (24/PATH-S/12518) grants.

Keywords: bone, spatially offset Raman spectroscopy, two-layer, Monte Carlo, optical properties

[Abstract:0330] [SERS/TERS/Plasmonics]

Silver Nanoparticles-Environmentaly Aged Blue Polypropylene Composite, Detection and Tracking of Micro- aAnd Nano- Sized Plastic Particles by SERS

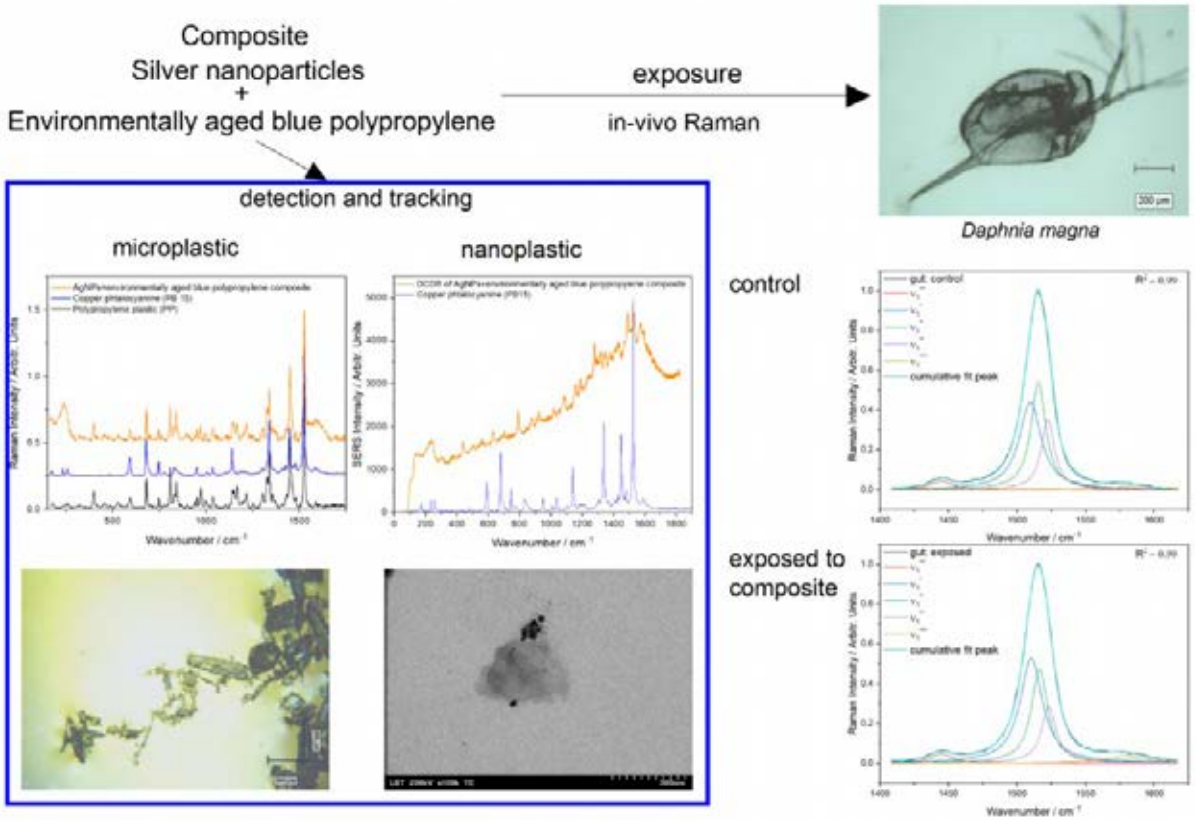
***Karlo Maškarić*[1], Ioana Cârdan[1], Matea Marelja[3], Ion Nesterovschi[1], Lucian Barbu-Tudoran[4], Tudor Tămaş[5], Codrut Costinas[2], Petra Tomurad[3], Anamaria Couți[2], Iuliana-Cornelia Sandu Poplăcean[2], Vera Slaveykova[3], Simona Cîntă Pînzaru[2]**

[1]*Biomolecular Physics Department, Babeş–Bolyai University, Kogălniceanu 1, RO, 400084, Cluj-Napoca, Institute for Research, Development and Innovation in Applied Natural Sciences, Babes-Bolyai University, Fantanele 30, Cluj-Napoca, Romania, National Institute for Research and Development of Isotopic and Molecular Technologies, Donat 67-103, Cluj-Napoca, 400293, Romania*
[2]*Biomolecular Physics Department, Babeş–Bolyai University, Kogălniceanu 1, RO, 400084, Cluj-Napoca, Institute for Research, Development and Innovation in Applied Natural Sciences, Babes-Bolyai University, Fantanele 30, Cluj-Napoca, Romania*
[3]*Environmental Biogeochemistry and Ecotoxicology, Department F.A. Forel for Environmental and Aquatic Sciences, Faculty of Sciences, University of Geneva, 66 Bvd Carl-Vogt 66, CH, 1211, Geneva, Switzerland*
[4]*Electron Microscopy Centre, Babeş-Bolyai University, Clinicilor 5-7, 400006 Cluj-Napoca, Romania*
[5]*Geology Department, Babeş-Bolyai University, Kogălniceanu 1, 400084 Cluj-Napoca, Romania*

Silver nanoparticles (AgNPs) are one of the most synthesized nanomaterials due to their wide use, and especially for the purpose of SERS. But, AgNPs are also very toxic, albeit their toxicity depending on the context; AgNPs properties, organisms interacting with it, and exposure scenarios. Another pollutant with complex impact on all levels of biological organization is plastic. It's effect are context dependent as well; polymer properties, concentration, chemical additives present. Inherent toxicity of AgNPs together with changing properties of plastic particles under environmental degradation, could lead to synergistic effect resulting in even higher toxicity compared to AgNPs alone. We synthesized AgNPs-blue polypropylene plastic (AgNPs-PP) composite using plastic recovered from the sea. The aims were: a) to develop a fast route to sensitive tracking using SERS as well as their intake/interaction in/with aquatic microorganisms, b) to read-out the synergic effect of both AgNPs and pigmented plastic, and c) to see to what extent the pigment is signalling from micro- down to nanoplastic-bearing pigment. *In vivo* Raman measurements were performed on *Daphnia magna* exposed to AgNPs-PP composite, to evaluate the possibility to detect it inside aquatic organisms. We demonstrate AgNPs-PP are detectable down to nano-sized particles, but their detection inside *D. magna* was not achievable within the standard ecotoxicological exposure conditions. However, *in vivo* Raman measurements of *D. magna* revealed carotenoid profile change as a response to acute toxicity of exposure to AgNPs-PP. Potential application of these composites and Raman and Raman-based methods in the ecotoxicological studies can add to knowledge about the synergistic ecotoxicological effects of the microplastic and nanoplastic with AgNPs on organisms.

Keywords: AgNPs-blue polypropylene, Cu-phtalocyanine (PB-15), Raman, SERS, in vivo, Daphnia magna

Graphical abstract



Detection and tracking of AgNPs - environmentally aged blue polypropylene plastic composite by Raman and SERS. Effect of Daphnia magna exposure on this composite in the Raman carotenoid profile.

Posters

[Abstract:0338] [Non-linear/Time-resolved]

Interfacial Water Organization in Glycocalyx Model Systems: Towards Understanding Blood-Brain Barrier Hydration Structure

***Dános Sebestyén Varga*[1], *Ilona Gróf*[1], *Lóránd Kelemen*[1], *Mária Anna Deli*[1], *Róbert Horváth*[2], *Zsuzsanna Heiner*[3], *András Dér*[1]**

[1]*Institute of Biophysics, HUN-REN Biological Research Centre, Szeged, Hungary*
[2]*Nanobiosensorics Laboratory, HUN-REN Centre for Energy Research, Budapest, Hungary*
[3]*Institute of Chemistry and School of Analytical Sciences Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany*

The blood-brain barrier (BBB) endothelial glycocalyx (GLX) maintains barrier integrity through mechanisms incompletely understood at the molecular level. While the GLX's role in selective permeability is established, the contribution of organized interfacial water remains unexplored. We hypothesize that oriented water structures within the GLX contribute steric and electrostatic barriers complementing tight junctions.

To investigate this, we developed a systematic approach using vibrational sum-frequency generation (VSFG) spectroscopy – a surface-selective technique probing oriented molecules at interfaces – combined with attenuated total reflection Fourier-transform infrared (ATR-FTIR) spectroscopy to study progressively complex GLX-relevant model systems.

We examined lipid monolayers at the air-water interface with GLX-relevant phospholipids and glycosphingolipids. VSFG measurements revealed distinct, oriented water signatures across the OH-stretching region, with spectral features varying with headgroup chemistry and surface pressure. Complementary studies on aqueous solutions of glycosaminoglycans (hyaluronic acid, chondroitin sulfate) showed concentration-dependent water orientation at the air-solution interface. Additionally, ATR-FTIR analysis quantified hydrogen bonding networks and identified specific carbohydrate-water interactions through characteristic spectral shifts.

These model system studies establish baseline interfacial water signatures for key GLX components. Our current work is progressing toward native membrane fragments to bridge the complexity gap between simplified models and the intact BBB endothelium. This systematic approach provides molecular-level insights into how GLX components organize interfacial water, potentially contributing to barrier function. Understanding these fundamental hydration structures may inform BBB pathophysiology in neurological disorders where GLX degradation occurs.

Keywords: vibrational sum-frequency generation, glycocalyx, blood-brain barrier, interfacial water, hydrogen bonding

[Abstract:0339] [SERS/TERS/Plasmonics]

Label-free SERS-based Profiling of Blood Serum Using Differentially Capped Gold Nanoparticles

***Septila Renata*[1], *Dragoș Ioan Olariu*[2], *Ciprian Paul Măirean*[1], *Vanda Gianina Moraru*[1], *Magdalena Aflori*[3], *Brindusa Dragoi*[4], *Rares Stiufiuc*[5]**

[1]*Nanotechnology Laboratory, TRANSCEND Department, Regional Institute of Oncology, 2-4 General Henri Mathias Berthelot, 700483 Iași, Romania*
[2]*Nanotechnology Laboratory, TRANSCEND Department, Regional Institute of Oncology, 2-4 General Henri Mathias Berthelot, 700483 Iași, Romania, Department of Physics of Polymers and Polymeric Materials, "Petru Poni" Institute of Macromolecular Chemistry, 700487 Iasi, Romania*
[3]*Department of Physics of Polymers and Polymeric Materials, "Petru Poni" Institute of Macromolecular Chemistry, 700487 Iasi, Romania*
[4]*Nanotechnology Laboratory, TRANSCEND Department, Regional Institute of Oncology, 2-4 General Henri Mathias Berthelot, 700483 Iași, Romania, Faculty of Chemistry, Alexandru Ioan Cuza University of Iași, 11 Bd. Carol I, 700506 Iași, Romania*
[5]*Nanotechnology Laboratory, TRANSCEND Department, Regional Institute of Oncology, 2-4 General Henri Mathias Berthelot, 700483 Iași, Romania, Department of NanoSciences, Institute for Biomedical Research- MedFUTURE, "Iuliu Hatieganu" University of Medicine and Pharmacy, 4-6 Pasteur Street, 400349 Cluj-Napoca,*

Cancer becomes a major public health problem and leading cause of death worldwide. Therefore, early detection of cancer and monitoring the disease during therapeutic treatment are highly required. Surface-enhanced Raman Spectroscopy (SERS) is an attractive modality for non-destructive analysis and quantification of biologically relevant molecules as it provides highly sensitive fingerprint molecular information. There are two approaches for SERS-based cancer detection, i.e., label-based and label-free. SERS primarily relies on noble metal (plasmonic) nanoparticles or rough metal surface as SERS substrate. The size, shape, material and configuration of nanoparticles greatly influence the SERS enhancements. Interestingly, the capping agent employed during synthesis of nanoparticle also gives effect to the SERS enhancement as detection tool, due to its laser transparency and binding affinity. Blood serum and plasma are the most common biological fluids used for cancer diagnosis and monitoring because they are rich in biochemical and biological information. Additionally, blood is less invasively collected at low cost.

In this work, we report label-free SERS profiling of blood serum using gold nanoparticles (AuNPs) with different capping agents used in their synthesis, cetyltrimethylammonium bromide (CTAB) and sodium citrate. Label-free SERS method is based on mutual interaction of analytes with SERS substrate, without need of Raman reporter and recognition molecule, allowing to detect intrinsic fingerprint of the molecule. Four different aspect ratios of gold nanorods and two different capped gold nanospheres, citrate@AuNPs and CTAB@AuNPs, have been synthesized and characterized using UV-vis, TEM and zeta potential. First, the measurement of uric acid, which is the dominant substance in serum based on most reported SERS measurements, was performed as a standard reference spectrum. Then the profiling of blood serum using SERS on citrate@AuNPs and CTAB@AuNPs has been compared.

Acknowledgements: This work was supported by a H2020 grant – ERA-Chair, no 952390.

Keywords: AuNPs, label-free method, SERS, serum

[Abstract:0343] [Industrial/Societal Applications]

Integrated approach based on Raman spectroscopy and chemometrics for the qualitative evaluation of wine and the monitoring of oenological processes

***Anna Lisa Gilioli*[1], *Alessio Sacco*[2], *Lorenzo Ferrero*[3], *Loretta Panero*[4], *Marco Lagori*[3], *Silvia Motta*[4], *Massimo Guaita*[4], *Andrea Mario Giovannozzi*[2], *Simone Giacosa*[3], *Antonella Bosso*[4], *Ettore Vittone*[1], *Andrea Mario Rossi*[2]**

[1]*Physics Department, University of Turin, Turin, Italy*
[2]*Istituto Nazionale di Ricerca Metrologica (INRiM), Turin, Italy*
[3]*Department of Agricultural, Forest and Food Sciences Department, University of Turin, Alba, Italy*
[4]*Consiglio per la ricerca in agricoltura e l'analisi dell'economia agraria (CREA), Asti, Italy*

Raman spectroscopy (RS) is a promising analytical technique for the rapid and non-destructive monitoring of key parameters in winemaking processes. The QualShelL project (which aims to implement new procedures for the qualitative evaluation of grapes and the monitoring of winemaking processes) explored the application of RS, combined with chemometric approaches, for the quantitative determination of compounds of oenological relevance in musts and wines (Figure 1).

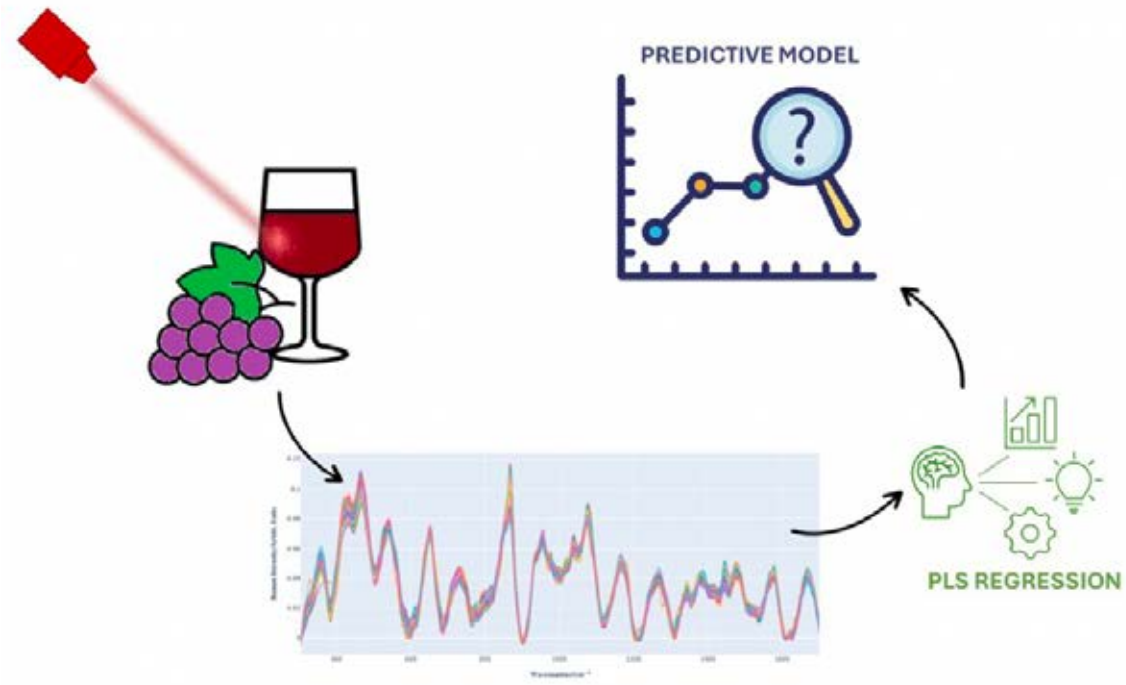
The first objective is to monitor malolactic fermentation (MLF), a process through which lactic bacteria convert malic acid into lactic acid and carbon dioxide to obtain stable wines characterised by greater balance and persistence in the mouth. Accurate control of this fermentation is essential to ensure product quality and compliance. Traditionally, this monitoring is carried out using high-performance liquid chromatography (HPLC); in this work, however, an alternative approach based on portable Raman spectroscopy is proposed to monitor the concentration of lactic acid in Nebbiolo must samples to produce Barolo wine. The Raman spectra acquired directly in the winery were processed and used as input for a PLS (partial least squares) regression model, trained using reference data obtained with HPLC. The method proved to be accurate and robust, leading to the determination of a predictive model characterised by an R^2=0.76 and RMSE = 0.22 g/L.

Subsequently, the same approach was applied to determine the total anthocyanins in wine, compounds that are fundamental to the organoleptic and antioxidant properties of red wines, particularly in terms of colour and sensory structure. The RS-PLS regression approach was applied to Barbera wine samples following a training phase based on ultraviolet-visible spectroscopy measurements. This methodology produced results comparable to traditional ones; in particular, it is characterised by: R^2=0.88 and RMSE =0.010 g/L.

The results demonstrate that Raman spectroscopy, thanks to its speed, non-destructive nature and the possibility of analysis directly in the vineyard or winery, is an effective tool for the quantitative monitoring of key parameters in winemaking processes, offering a practical, fast and less expensive alternative to traditional analytical methods.

Keywords: Raman spectroscopy, PLS Regression, malolactic fermentation, anthocyanins.

Figure 1



Raman-PLS regression approach

Posters

[Abstract:0346] [Coherent Raman Imaging]

A Fiber-Compatible Fiber Optical Parametric Oscillator for Stimulated Raman Scattering Microscopy

***Qingcheng Song*[1], *Shun Takahashi*[1], *Norihiko Nishizawa*[3], *Shotaro Kitajima*[3], *Yasuyuki Ozeki*[2]**

[1]*Department of Electrical Engineering and Information Systems, The University of Tokyo, Tokyo, Japan*
[2]*Department of Electrical Engineering and Information Systems, Research Center for Advanced Science and Technology, The University of Tokyo, Tokyo, Japan*
[3]*Department of Electronics, Nagoya University, Nagoya, Japan*

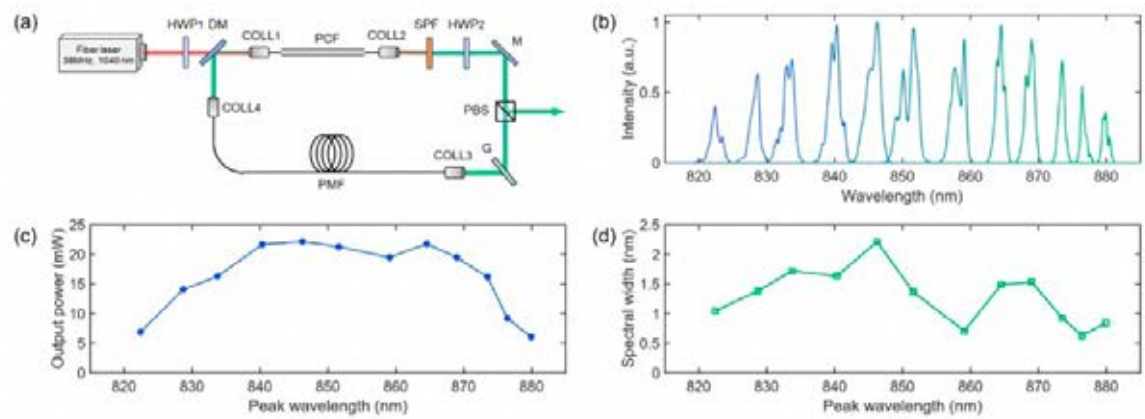
Stimulated Raman scattering (SRS) microscopy is a label-free vibrational imaging technique that enables chemically specific imaging with high spectral resolution. Accessing different vibrational modes requires tuning the frequency difference between pump and Stokes beams, which motivates the development of high performance pulsed light sources. Fiber optical parametric oscillators (FOPOs) provide an attractive approach due to their broad tuning capability and potential in compact configuration. However, fully fiber-based FOPO implementations remain limited. In addition, previously demonstrated FOPO-based SRS sources often suffer from higher intensity noise than fiber laser or optical parametric oscillators, which degrades signal-to-noise ratio and typically necessitates balanced detection in imaging systems. In our previous study, we developed a widely tunable FOPO synchronized with a low-noise Ti:sapphire laser for low-noise SRS microscopy. Nevertheless, the FOPO was implemented with free-space optical components, resulting in a relatively large system footprint and strict alignment requirements.

In this work, we experimentally demonstrate a fiber-compatible FOPO featuring a reduced system footprint and improved robustness (Fig. 1). The FOPO is pumped by a high-power fiber laser, in which a photonic crystal fiber (PCF) generates frequency-upshifted signal light through four-wave mixing. To improve mechanical stability, a pair of fiber collimators is fusion-spliced to both ends of the PCF. A diffraction grating inside the cavity provides wavelength selection and spectral filtering, enabling a narrow spectral linewidth suitable for SRS applications. A 3.8-m long polarization-maintaining fiber is employed to build up a cavity with a fixed repetition rate of 38 MHz. The integration of fiber components reduces the reliance on free-space optical elements, leading to improved mechanical stability and a more compact system architecture. The measured output performance is shown in Fig. 1(d)-(d). The FOPO delivers tunable output over a wavelength range of 822–880 nm with an output power of ~22 mW and a spectral width of ~2 nm.

In the future, the FOPO will be synchronized with a 76 MHz low-noise Ti:sapphire laser for low-noise SRS microscopy. The demonstrated fiber-compatible architecture represents a key step toward all-fiber FOPO, enabling more compact and robust nonlinear optical sources for nonlinear imaging and spectroscopic applications.

Keywords: Tunable laser, fiber optical parametric oscillator, photonics crystal fiber, stimulated Raman scattering microscopy

Figure 1. Schematic setup and performance of FOPO.



(a) Schematic setup of FOPO cavity. HWP: half-wave plate, DM: dichroic mirror, PCF: photonic crystal fiber, SPF: short-pass filter, M: mirror, PBS: polarizing beam splitter, G: grating, PMF: polarization-maintaining fiber, COLL: fiber collimator. (b)-(d) Measured output spectra, output power and spectral width of FOPO.

[Abstract:0350] [Industrial/Societal Applications]

Nanostructured SERS Substrates Engineered via Colloidal Lithography for Environmental Nanoplastics Detection

***Ioana Cârdan*[1], *Ana Maria Mihaela Gherman*[2], *Lucian Barbu-Tudoran*[2], *Septimiu Tripon*[2], *Denisa Cuibus*[2], *Serena Ducoli*[3], *Stefania Federici*[3], *Simona Cîntă Pînzaru*[4], *Cosmin Farcău*[2]**

[1]*Faculty of Physics, Babeş-Bolyai University, Cluj-Napoca, Romania, Isotopic and Molecular Technologies Department, National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania*
[2]*Isotopic and Molecular Technologies Department, National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania*
[3]*Department of Mechanical and Industrial Engineering, University of Brescia, Brescia, Italy*
[4]*Faculty of Physics, Babeş-Bolyai University, Cluj-Napoca, Romania*

Nanoplastics (NPs), defined as plastic particles smaller than 1 μm, have recently attracted global attention due to their accumulation in the environment and the significant challenges associated with their detection and tracking. Beyond their small size, the detection of environmental NPs poses additional difficulties due to their diverse heterogeneous composition and contamination. Moreover, prolonged exposure to various environmental factors can further modify their physical and chemical properties, making detection even more complex. Therefore, the challenges occurring in accurately identifying and quantifying these particles has driven increasing interest in the development of efficient analytical methods.

In this context, surface-enhanced Raman scattering (SERS) spectroscopy has emerged as a promising technique for NP detection, applicable to both standard and environmentally derived NPs. While SERS is well established for molecular analytes, its use in NP detection remains under active development, particularly for environmental NPs, which present unique challenges.

In this study, we address environmental NPs detection using customized nanostructured SERS substrates engineered based on our recent findings on substrate design, emphasizing the importance of substrate morphology and the physical features of nanoplastics. To this end, nanostructured SERS substrates with different morphologies were fabricated using colloidal and soft lithography, and their morphology and optical response were characterized. Their enhancement performance was first assessed using standard nanoplastics, followed by more realistic nanoplastic samples, true-to-life NPs. Environmental NPs, consisting of blue NPs degraded under aquatic conditions, were subsequently detected by combining the SERS enhancement of the customized substrates with the Resonance Raman (RR) signal of copper phthalocyanine (CuPc), a pigment commonly found in blue plastics. To further understand how substrate morphology and the heterogeneous physical characteristics of the environmental NPs influence SERS enhancement, we also performed finite-difference time-domain (FDTD) simulation of the field enhancement in differently sized and shaped nanoplastics on various SERS substrates.

This study demonstrates the potential of morphologically tailored SERS substrates for detecting environmental nanoplastics and provide valuable insights into both the advantages and limitations of SERS-based approaches for environmental NPs detection and analysis.

Keywords: nanoplastic, SERS detection, nanostructured substrate, colloidal lithography, optimization

Posters

[Abstract:0358] [Non-linear/Time-resolved]

Structure of the hydrated electron elucidated by the synergy of polarized-resolved FSRS spectroscopy and DFT computations

Ewa Pastorczak[1], Karolina Skała[2], Andrzej Sobolewski[3], Marcin Pastorczak[2]

[1]Institute of Physics, Lodz University of Technology, ul. Wólczańska 217/221, 93-590 Łódź, Poland
[2]Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland
[3]Institute of Physics, Polish Academy of Sciences, 02-668 Warsaw, Poland

Determining the structure of the hydrated electron ($e^-(H_2O)$) is a long-standing problem in chemistry, with multiple structures proposed over the decades. A critical advance in the field came with the observation of the band at around 3170 cm^{-1} in the water's OH stretch interacting with a solvated electron [Mizuno & Tahara, J. Phys. Chem. 2003, Tauber & Mathies JACS 2003].

In the presented work, we generated the $e^-(H_2O)$) with a strong 2 ps pulse at 515 nm that simultaneously acted as a Raman pump in the FSRS (fs stimulated Raman scattering) experiment. We probed the system with varied pump pulse power and FSRS polarization (VV/HV). We observed a nonlinear increase in the intensity of the band around 3200 cm^{-1} with the pump power. The band ingrowth was also associated with beam filamentation and supercontinuum generation in water, at the highest energies. We thus assigned the band to the $e^-(H_2O)$) presence. The polarization-resolved studies showed that the ~3200 cm^{-1} band is strongly polarized (see Fig. 1).

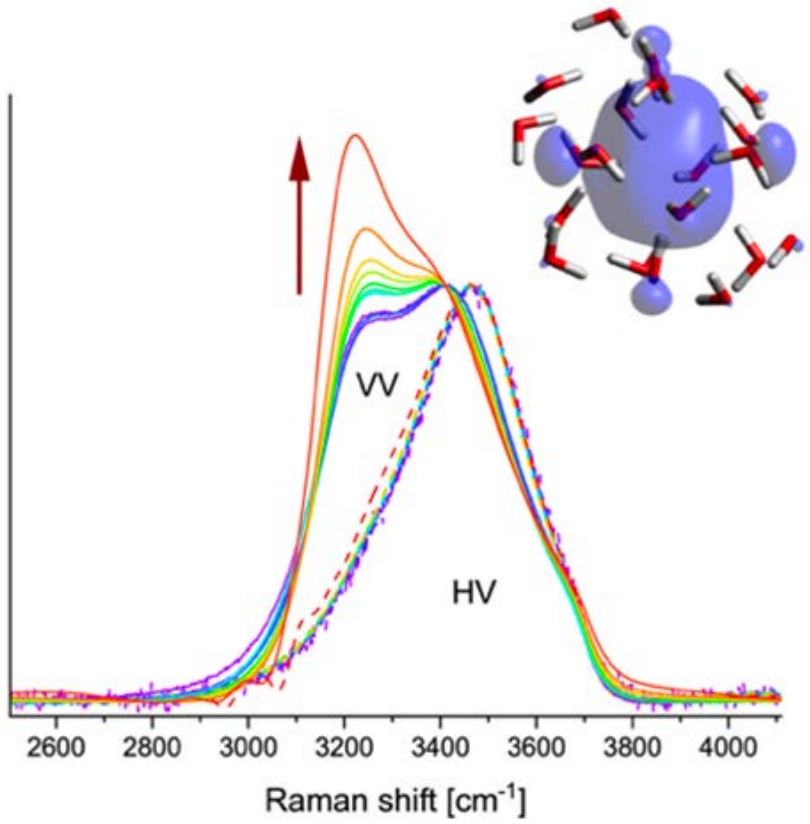
Complementary density-functional theory computations allowed us to find minimum-energy anionic water cluster structures with a localized electron in the center (cf. Fig. 1) whose spectra qualitatively reproduce the experimental results and the appearing band is related to an OH-group bond stretching enhanced by the presence of the spare electron.

The prospect of this work is to study electron–scavenger interactions in water, e.g., using atomically precise metal nanoclusters with multiple redox potentials as electron scavengers.

This work was supported by the Polish National Science Center (NCN OPUS grant no. 2021/43/I/ST4/01411).

Keywords: hydrated electron, polarized FSRS, DFT

Fig.1



The normalized VV(solid line) and HV (dashed line) FSRS spectra of liquid H2O vs 515 nm pump pulse energy (left) and the computed structure of a 20-molecule anionic water cluster with a singly-occupied molecular orbital isosurface (right).

[Abstract:0364] [Non-linear/Time-resolved]

A Simple and Adaptable Solution for Measuring Time Traces from Sub-Picosecond to Sub-Microsecond in FSRS Spectroscopy

Hector Rodriguez, Sanat Kumar Mahankudo, Karolina Skała, Gonzalo Angulo

Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland

A typical problem with time resolved spectroscopies is the mismatch between experimental data recorded with different time resolutions. Interrogating a chemical or physical system with a high temporal resolution comes at the cost of a limited maximum observation time imposed by mechanical delay lines (few ns). On the other hand, the experimental conditions, like pump energy, spectral coverage and others, in longer time techniques which might expand up to ms, are usually so different from those in the former short-time methods, that serious problems are encountered when trying to merge both [Eads et al. J Chem. Phys. 93, 1990]. In FSRS research this problem is particularly vital regarding studies of photoactive proteins, where the response of chromophores is usually in the picoseconds' timescale, while that of proteins in hundreds of nanoseconds. Many experimental solutions have been proposed to perform measurements up to long delay times with high temporal resolution, but they are usually very expensive and complex to implement. [Bredenbeck et al., Rev. Sci. Inst.,75, 2004]

We show a technical solution to reduce the complexity and costs to achieve exactly this goal, enabling performing time-resolved spectroscopy such as transient absorption experiments or FSRS up to several hundreds of ns with an instrument response function below 200 fs.

In the poster, the details of the experimental set-up will be shown along with some example experiments.

Keywords: FSRS, Time-resolved, long time delay scanning, technical development

[Abstract:0366] [SERS/TERS/Plasmonics]

Influence of Gold Nanoparticle Morphology on SIERS/SERS Enhancement on Silicon Substrates with V-Shaped Microchannels

***Italo Odone Mazali*, Deysiane Alves Lima Dos Santos, Anerise de Barros, Fernando Aparecido Sigoli**

Institute of Chemistry, University of Campinas, Campinas, SP, Brazil

Surface-Enhanced Raman Spectroscopy (SERS) is widely used for the detection of molecules at low concentrations due to the amplification of the Raman signal promoted by plasmonic metallic nanostructures. Recently, our group demonstrated that silicon substrates containing V-shaped cavities (Si-V) can promote Raman signal enhancement through the SIERS effect (Shape-Induced Enhanced Raman Scattering). In this context, the present work investigates the influence of gold nanoparticle morphology on the efficiency of the SIERS effect using nanospheres (AuSph) and nanocubes (AuNCs). The AuSph and AuNCs were synthesized following methods previously established in our research group. Subsequently, 20 μL of these nanoparticle suspensions were deposited onto Si-V substrates and dried at room temperature (~25 °C). Afterwards, 10 μL of thiram fungicide solutions at different concentrations were added to the substrates. For comparison purposes, the same procedure was carried out using flat silicon substrates (Si-flat). After deposition, the efficiency of the SIERS/SERS platforms was evaluated. Preliminary results show that AuSph on Si-V substrates enabled the detection of the fungicide thiram in the range of 10^{-2} to 10^{-9} M, whereas on Si-flat substrates detection occurred between 10^{-2} and 10^{-6} M. Comparatively, Si-V substrates presented relative enhancement factors between 1.92 and 3.27 times higher compared to Si-flat. For AuNCs, detection on Si-V was even more sensitive, reaching concentrations from 10^{-2} to 10^{-17} M, in contrast to 10^{-2} to 10^{-8} M observed for Si-flat. In this comparison, the relative enhancement factors ranged from 1.24 to 15.08 times for the Si-V substrates. Overall, these results demonstrate that Si-V substrates promote greater Raman signal enhancement compared to Si-flat substrates, regardless of nanoparticle morphology. Furthermore, AuNCs showed superior performance and, when combined with Si-V substrates, enabled ultrasensitive detection of thiram, highlighting the strong potential of this SIERS/SERS platform for trace-level detection.

Keywords: Gold nanoparticles, SIERS, SERS, thiram detection

[Abstract:0376] [Materials]

Representative Reference Materials for Microplastic Analysis

***Nicolas Coca Lopez*[1], *Teagan Horan*[2], *James Roussie*[2], *Robert Fabinski*[2], *Miguel A. Bañares*[1], *Raquel Portela*[1], *Andrew B. Gray*[3], *Win Cowger*[4]**

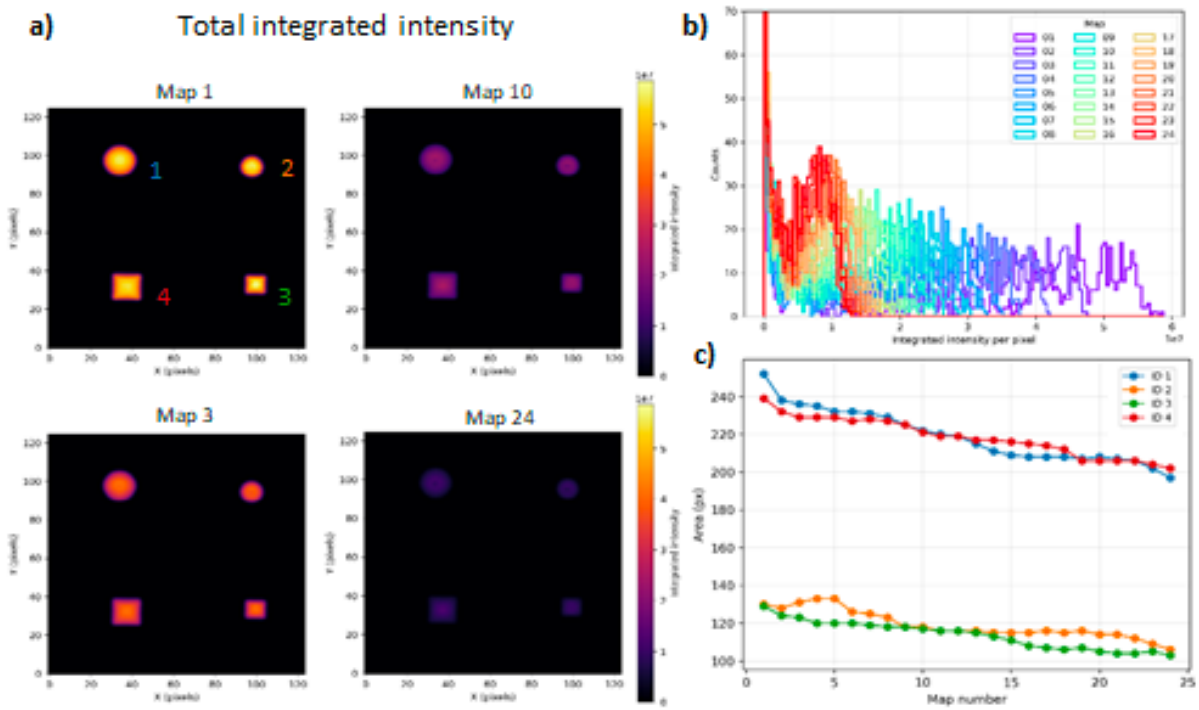
[1]*Instituto de Catalisis y Petroleoquimica (ICP), CSIC, Madrid, Spain*
[2]*SiMPore Inc., West Henrietta, NY, USA*
[3]*Department of Environmental Sciences, University of California, Riverside, CA, USA*
[4]*The Moore Institute for Plastic Pollution Research, Long Beach, CA, USA*

Micro and nanoplastics (MNPs) pose a complex ecological and health issue due to their diverse morphologies, chemical compositions, and transformation behaviours across freshwater, marine, and terrestrial ecosystems. Accurate and conclusive MNP analyses hinge on representative reference materials, harmonized protocols, validated instruments, and robust workflows. While Raman spectroscopy has emerged as a reference technique for chemical identification, the field lacks standardized reference materials, particularly for characterizing particles below the critical 20-micrometer threshold. In this work, we present the development of representative reference samples designed to test the technical limits of Raman microspectroscopy. Reference samples consisting of silicon substrates with lithographically defined polymer features were prepared with known, varying shapes and sizes in the micrometer range down to 10 micrometers. These well-defined and precisely located MNP mimics allow for a detailed assessment of particle microspectroscopic measurement bias and instrument-to-instrument variability based on photoluminescence emission, facilitating instrument validation. Map binarization and particle area calculation was studied under different sample and measurement distortions including photobleaching (Figure 1), defocusing, and for different parameters as laser power and integration time, showing their suitability as a reference material. Complementary tests with commercial, well-characterised water suspensions of polypropylene microbeads with 20 micrometers diameter were performed to evaluate filtration recovery efficiencies and hyperspectral analysis. By benchmarking micro Raman instruments performance against these reference lithographic and filtered materials, we establish the foundations for a metrological framework in particulate monitoring. This initiative contributes to a more cohesive infrastructure that supports the long-term comparability and transferability of plastic pollution assessment and has applicability in fields as pharmaceutics and forensics.

Keywords: Particle analysis, environmental monitoring, metrology, validation protocol

Posters

Photobleaching of lithographically defined microplastic particles for threshold estimation



a) Photoluminescence total integrated intensity maps after being scanned 1, 3, 10 and 24 times. b) Total integrated intensity histograms. c) Calculated area of the four particles.

[Abstract:0377] [Coherent Raman Imaging]

Cellular Senescence Profiling by Multiplex CARS Spectroscopic Imaging

***Ayana Kotegawa*[1], *Rina Kunishige*[2], *Ryo Suzuki*[1], *Masayuki Murata*[2], *Fumi Kano*[2], *Hideaki Kano*[1]**

[1]*Faculty of Science and Technology, Keio University, Yokohama, Japan*
[2]*Multimodal Cell Analysis Collaborative Research Cluster, Institute of Science Tokyo, Yokohama, Japan*

Cellular senescence is characterized by irreversible cell cycle arrest and plays a central role in aging-related functional decline. Quantitative, label-free detection of senescent cells is therefore essential for evaluating tissue deterioration. In this study we explore Raman spectroscopic indicators of cellular senescence based on intrinsic vibrational signatures without exogenous staining.

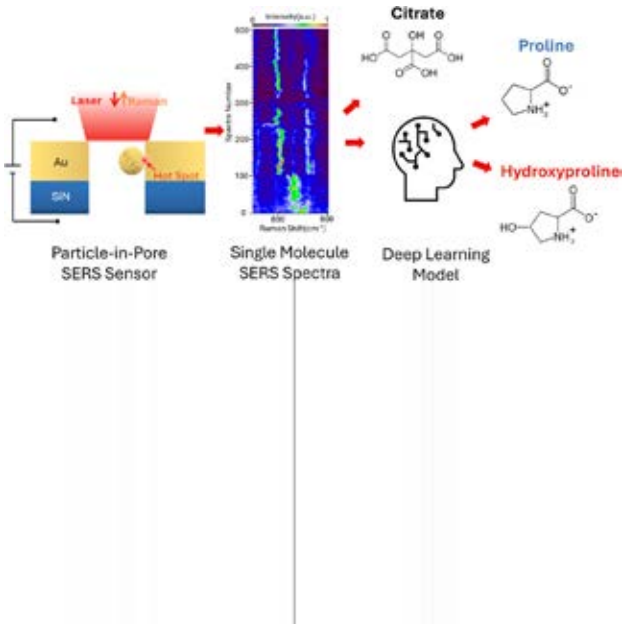
Senescence was induced in human fibroblasts using a mitosis-skip protocol [Johmura et al., Science 371, 265, (2021), Johmura et al., Molecular Cell 55, 73, (2014)]. Cells synchronized at G2/M with RO-3306 were treated with Nutlin-3a to bypass mitosis, followed by a 20-day maturation period. Early-passage cells were used as controls. Label-free single-cell imaging was performed using multiplex coherent anti-Stokes Raman scattering (CARS) microscopy [Masaki et al., Anal. Chem. 97, 28, 15299-15309 (2025)].

A characteristic Raman band around ~713 cm^{-1} was observed in the cytoplasm of senescent cells (n=7/41) (Fig. 1(a)). Comparison with spectra of phosphatidylcholine and sphingomyelin suggests that this signal originates from the choline headgroup of phospholipids (Fig. 1(b)). The image generated from the 713 cm^{-1} band, constructed from the amplitude of a Gaussian fit to the spectrum averaged over a 2.5 μm surrounding region, shows strong correspondence with the fluorescence image of the lysosomal marker LAMP2 (Fig. 2), indicating an association with lysosomal accumulation and membrane reorganization in senescent cells.

These results indicate that cytoplasmic lipid-related vibrational signatures have the potential to serve as reliable label-free indicators of cellular senescence. This study establishes a spectroscopic basis for detecting senescent states using multiplex CARS spectroscopic imaging and supports further development toward quantitative evaluation of cellular aging process.

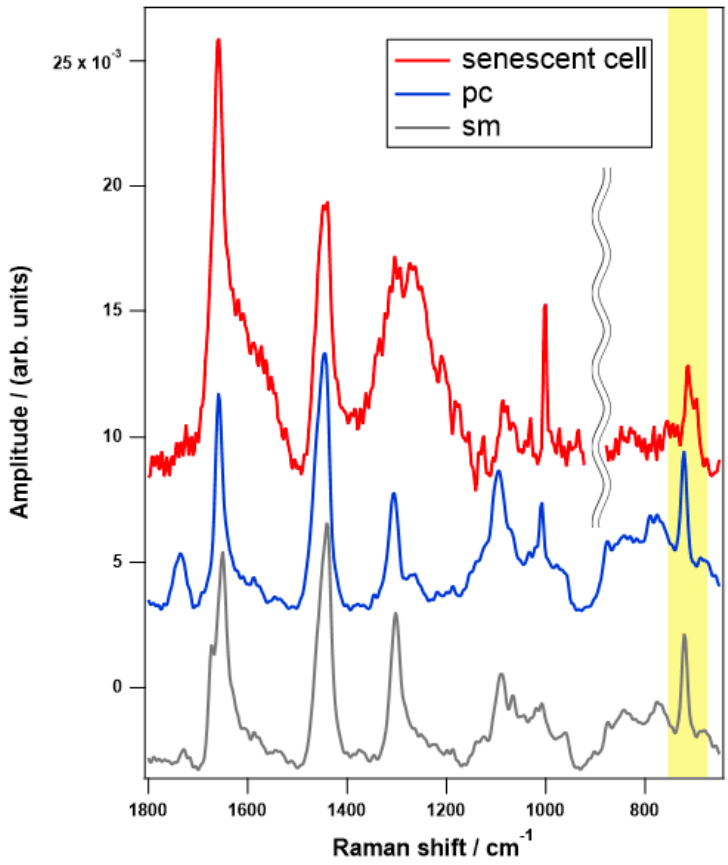
Keywords: CARS, Microscopy, Senescent cells

Figure 1. (a)



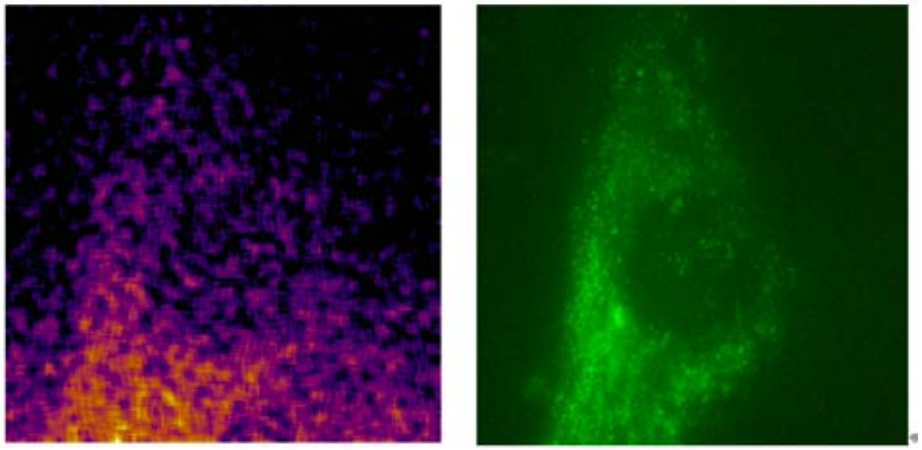
CARS image highlighting cellular morphology around 2930 cm-1

Figure 1. (b)



Comparison of cytoplasmic Raman spectra in senescent cells at the region indicated by the green square with reference lipid spectra. Baseline correction has been applied.

Figure 2



CARS image around 713 cm^{-1} (left) and corresponding LAMP2 fluorescence image (right). The CARS image is constructed from the amplitude of a Gaussian fit to the spectrum averaged over a 2.5 μm surrounding region.

Posters

[Abstract:0383] [SERS/TERS/Plasmonics]

Excitation Wavelength-Dependent Variability of Methylene Blue SERS Spectra on Silver Substrates

***Matěj Kmetík*[1], *Ivan Kopal*[2], *Král Martin*[3], *Marcela Dendisová*[3]**

[1]*Department of Physical Chemistry, University of Chemistry and Technology, Prague, Czech Republic, Analytical Laboratory, Institute of Organic Chemistry an Biochemistry of the CAS, Prague, Czech Republic*
[2]*Institute of Photonics and Electronics, Czech Academic of Sciences, Prague, Czech Republic, Department of Physical Chemistry, University of Chemistry and Technology, Prague, Czech Republic*
[3]*Department of Physical Chemistry, University of Chemistry and Technology, Prague, Czech Republic*

Surface-enhanced Raman scattering (SERS) has undergone remarkable development over the past five decades; however, its practical application still involves significant complexity. The resulting SERS signal arises from the interplay of multiple enhancement mechanisms and is influenced by numerous experimental parameters, including excitation wavelength, substrate material, molecular orientation, temperature, pH, and substrate aging. These contributions are commonly divided into two principal mechanisms: the electromagnetic (EM) mechanism, governed by local field enhancement and strongly dependent on excitation wavelength and plasmonic substrate, and the chemical mechanism (CM), which involves changes in the electronic structure of the adsorbed molecule, including charge transfer (CT) processes and molecule–surface interactions.

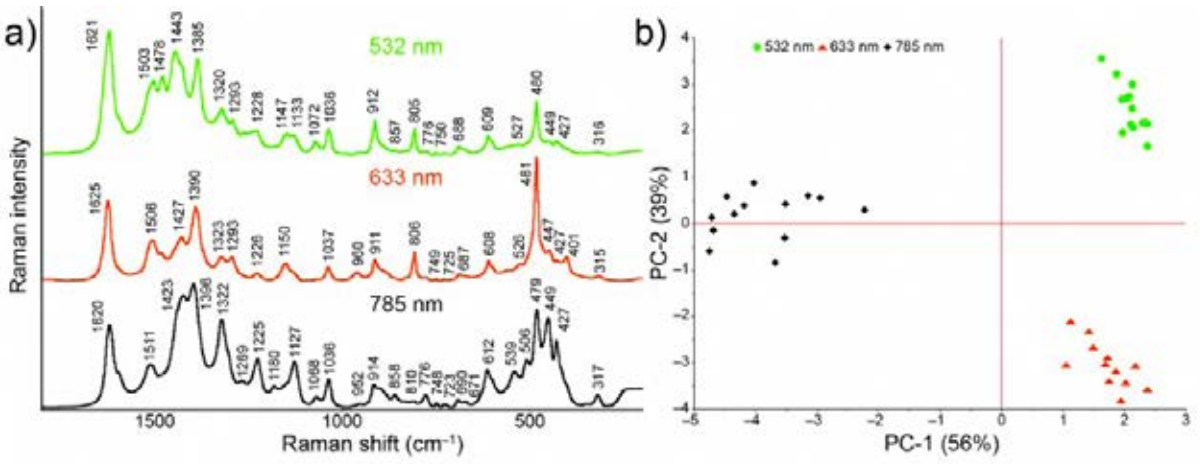
Methylene blue (MB) represents a widely used model analyte due to its chemical relevance and well-defined absorption band around 660 nm, enabling surface-enhanced resonance Raman scattering (SERRS). However, this resonance condition also introduces complications, such as photochemical transformations (e.g., N-demethylation) under visible excitation. Additionally, plasmon-induced catalysis may alter reaction pathways, and CT interactions between MB and the metal surface can further modify spectral features. While these effects can enhance sensitivity and lower detection limits, they also increase the risk of spectral misinterpretation.

In this work, we extend our previous investigations of MB SERS variability on Au and Cu substrates by focusing exclusively on silver-based systems (Ag-SERS). The variability of MB SERS spectra was systematically studied using multiple excitation wavelengths (532, 633, 785, and 1064 nm), covering a broad spectral range from visible to near-infrared. Particular attention was paid to the dependence of spectral features on excitation wavelength and to the role of photoinduced and plasmon-driven chemical transformations. Wavelenght-dependent measurements involving repeated laser exposure were employed to monitor potential changes in the deposited species (Figure 1, a) SERS spectra of MB measured with different excitation waveleghts b) Scatter plot of PCA scores).

The obtained results provide deeper insight into the interplay between EM and CM contributions, as well as into wavelength-dependent surface processes. This study highlights both the analytical potential and the inherent complexity of SERS and contributes to a more reliable interpretation of SE(R)RS spectra of MB and related systems.

Keywords: SERS, methylenblue, silver substrate, photochemistry

a) SERS spectra of MB measured with different excitation waveleghts b) Scatter plot of PCA scores



[Abstract:0385] [Industrial/Societal Applications]

Adaptive Confocal Raman Imaging for Rapid Spatial Characterization of Pharmaceutical Solids

Hajar Elazri

HORIBA France SAS, Palaiseau, France

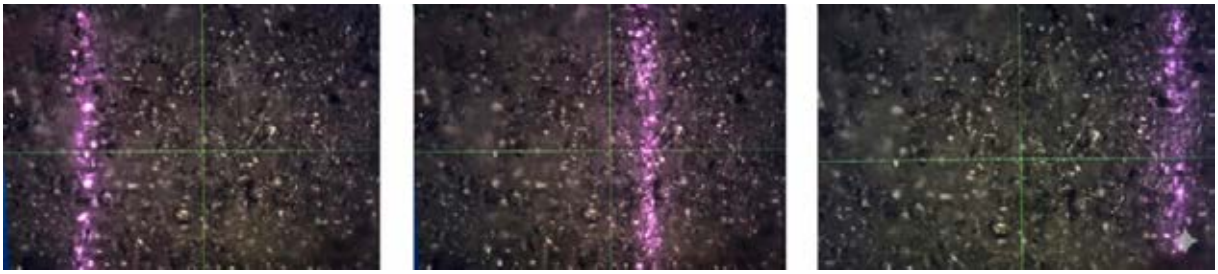
Pharmaceutical solids often combine chemical heterogeneity with sensitivity to prolonged laser exposure, local heating, and photoinduced transformations. These constraints limit the applicability of conventional dense Raman mapping strategies based on static, pointbypoint acquisition.

In this work, adaptive sampling combined with fast confocal Raman beam scanning is presented as an efficient alternative for microscale chemical characterization. Adaptive acquisition dynamically prioritizes spectrally informative regions, allowing chemically meaningful spatial contrast to emerge at early stages of measurement and significantly reducing overall acquisition time. Fast beam scanning further limits local energy density by avoiding long laser dwell at a single position while maintaining confocal imaging performance.

Applied to heterogeneous pharmaceutical solids, this combined approach enables rapid visualization of compositional domains and interfaces while mitigating sample alteration associated with extended laser exposure. Adaptive confocal Raman imaging thus provides a balanced framework for achieving chemical specificity, spatial resolution, acquisition efficiency, and sample preservation in pharmaceutical solidstate analysis.

Keywords: Adaptive sampling, Beamscanning Raman, Lasersensitive materials

Dynamic beam-scanning of a pharmaceutical tablet



[Abstract:0387] [Biology/Biomedicine]

Site-Specific UVRR Investigation of Maltose-Binding Protein Using 5-CN-Trp as a Selective Probe

***Wonki Son*[1], *Adarshi P. Welegedara*[2], *Luca Supovec*[1], *Thomas Huber*[2], *Gottfried Otting*[2], *Sebastian Schlücker*[1]**

[1]*Department of Chemistry, University of Duisburg-Essen, Essen, Germany*
[2]*Research School of Chemistry,The Australian National University, Canberra, Australia*

Elucidating protein binding mechanisms in physiological environments is crucial for understanding biological functions. While conventional techniques such as X-ray crystallography and cryo-EM provide high-resolution structural information, they generally offer static snapshots and do not always reflect protein behavior under aqueous conditions. On the other hand, methods such as fluorescence and circular dichroism often lack detailed structural specificity, whereas NMR can have practical limitations in sample preparation and measurement conditions. To address these challenges, Raman spectroscopy offers a powerful, non-destructive approach for analyzing proteins in their native aqueous environment.

However, sensitivity and selectivity are major challenges: spontaneous Raman signals are inherently weak and are often convoluted by the complex protein matrix. Ultraviolet Resonance Raman (UVRR) spectroscopy overcomes these limitations by selectively enhancing the vibrational modes of aromatic amino acids such as tryptophan. This selective enhancement suppresses much of the spectral background and provides a sensitive probe of the local microenvironment.

In this study, we employed UVRR to investigate maltose binding in a series of 5-CN-Trp-labeled Maltose-Binding Protein (MBP 5CNW) mutants. Using 5-CN-Trp as a selective resonant probe at different positions, we monitored localized spectral changes in the C≡N stretching mode upon ligand interaction. Among the tested variants, the MBP 340 mutant exhibited the most pronounced spectral shift, indicating that it is the most responsive probe position for tracking maltose binding. Based on this screening, MBP 340 was selected for titration experiments, in which the concentration-dependent peak shifts were analyzed to estimate the binding constant (Kd).

These results demonstrate that site-specific UVRR with 5-CN-Trp is an effective and quantitative tool for monitoring ligand-induced local environmental changes and for identifying responsive probe positions in complex protein systems.

Keywords: UV resonance Raman, 5-cyanotryptophan, protein–ligand interactions

Posters

[Abstract:0393] [Novel Approaches]

Towards FAIR Raman and IR Spectroscopy: A Minimal Metadata Framework

***Jamile Jafari*[1], *Shuxia Guo*[1], *Oleg Ryabchykov*[1], *Darina Storozhuk*[1], *Thomas Bocklitz*[2]**

[1]*Photonic Data Science, LeibnizInstitut für Photonische Technologien (IPHT), Jena, Germany*
[2]*Institute of Physical Chemistry (IPC) and Abbe Center of Photonics (ACP), Friedrich Schiller University Jena, Jena, Germany*

Raman spectroscopy is a powerful, non-destructive technique widely used for molecular identification and structural characterization in chemistry, materials science, and life sciences. Complementary to Raman, infrared (IR) spectroscopy provides additional insight into molecular vibrations and chemical composition. Various experimental approaches exist, including spontaneous Raman, resonance Raman (RRS), and surface-enhanced Raman spectroscopy (SERS), as well as Fourier-transform infrared (FTIR), attenuated total reflectance (ATR), and transmission and reflection IR modes. These methods differ in signal generation, measurement configurations, and experimental setups, enabling applications from bulk analysis to nanoscale and spatially resolved studies.

Despite this broad applicability, the lack of standardized and minimal metadata reporting remains a major challenge. Experimental results are highly sensitive to instrumental settings, acquisition parameters, calibration procedures, and data processing steps. Without consistent documentation, reproducibility is compromised, cross-study comparability is limited, and data reuse becomes difficult. This limitation also hinders alignment with FAIR data principles (Findable, Accessible, Interoperable, Reusable), which increasingly guide modern scientific data management. While existing standardization efforts provide partial solutions, they are often domain-specific and do not fully address methodological diversity.

In this work, we propose a generalized schema for minimal metadata reporting, covering both Raman and IR techniques. The framework captures essential experimental details across the full workflow, from excitation or illumination to detection and data processing. It combines a common core of metadata elements with method-specific modules for individual techniques, enabling both consistent documentation and technique-dependent detail. This approach supports improved reproducibility, interoperability, and FAIR-compliant data practices.

• Funding

This work is supported by the BMFTR, funding program Photonics Research Germany (13N15466 (LPI-BT1-FSU), 13N15708 (LPI-BT3-IPHT)) and is integrated into the Leibniz Center for Photonics in Infection Research (LPI). The LPI initiated by Leibniz IPHT, Leibniz-HKI, Friedrich Schiller University Jena, and Jena University Hospital is part of the BMFTR national roadmap for research infrastructures. The project is co-funded by the DFG (NFDI4Chem, 441958208).

Keywords: Raman spectroscopy, Infrared spectroscopy, Metadata, FAIR

Posters

[Abstract:0394] [SERS/TERS/Plasmonics]

Single-Molecule SERS for DNA Nucleobase Classification Using 1D CNN: A Comparative Study with Machine Learning Methods

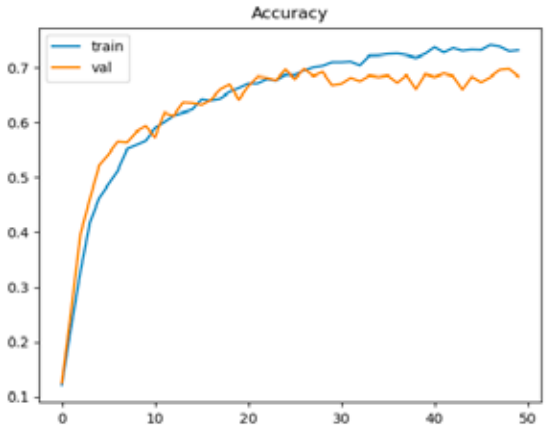
***Enock Adjei Agyekum*[1], *Yingqi Zhao*[3], *Kuo Zhan*[3], *Jian An Huang*[2], *Shuai Li*[1]**

[1]*The Biomimetics and Intelligent Systems (BISG) research unit, Faculty of Information Technology and Electronic Engineering, University of Oulu, 90220 Oulu, Finland*
[2]*Research Unit of Health Sciences and Technology, Faculty of Medicine, University of Oulu, 90220 Oulu, Finland; Research Unit of Disease Networks, Faculty of Biochemistry and Molecular Medicine and Biocenter Oulu, University of Oulu, 90220 Oulu, Finland*
[3]*Research Unit of Health Sciences and Technology, Faculty of Medicine, University of Oulu, 90220 Oulu, Finland; Biocenter Oulu, University of Oulu, 90220 Oulu, Finland*

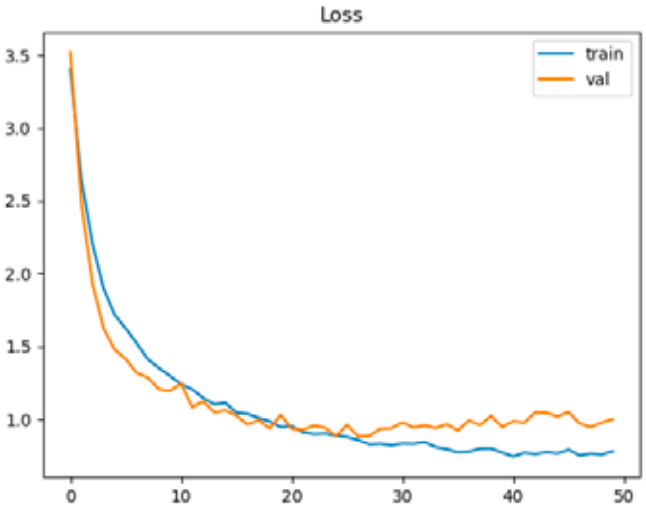
Surface-enhanced Raman spectroscopy (SERS) is a powerful analytical method known for its ability to detect and identify molecular species at very low concentrations, even down to single molecules. A key application of SERS is the accurate classification of DNA nucleobases, which is essential for advancing label-free DNA sequencing technologies. These technologies promise to simplify workflows and reduce costs by eliminating the need for fluorescent or radioactive labels. Additionally, SERS plays a critical role in developing sensitive biosensing platforms for medical diagnostics, environmental monitoring, and forensic analysis. Integrating SERS into automated molecular diagnostic systems could enhance the speed, accuracy, and reliability of disease identification and genetic screening, improving healthcare outcomes. This study presents a data-driven approach for classifying fifteen DNA nucleobases using single-molecule SERS spectral data with a one-dimensional convolutional neural network (1D CNN). The 1D CNN automatically extracts discriminative spectral features, eliminating the need for manual feature engineering, and performs well even with noisy data. The model demonstrated an overall classification accuracy of about 70% and impressive one-vs-rest area under the curve (AUC) values between 0.92 and 1.00, outperforming traditional machine learning algorithms like SVM, KNN, MLP, RF, LR, and LDA, which achieved accuracies below 50%. Despite their lower overall accuracy, classical models showed moderate AUC values (0.59 to 0.99), indicating some ability to differentiate classes. The findings suggest that deep learning is more effective in identifying complex patterns in SERS data, offering a robust methodology for nucleobase identification and enhancing real-time, label-free molecular analysis in biosensing applications.

Keywords: Single molecule, CNN, SERS

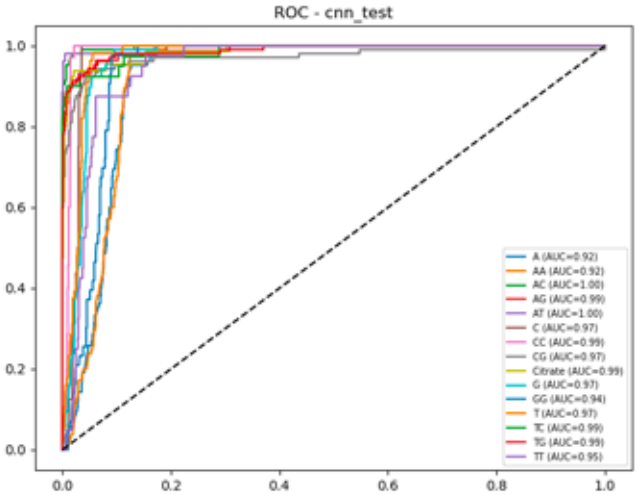
Accuracy curves of IDCNN model



Loss curves of the IDCNN model



ROC curves for IDCNN model



[Abstract:0404] [Non-linear/Time-resolved]

Deep Learning Enhanced Time Domain Raman Spectroscopy

Giovanni Batignani, Pietro Lussana, Emanuele Mai, Neethish Madathiparambil Mohanan, Stefano Giagu, Tullio Scopigno

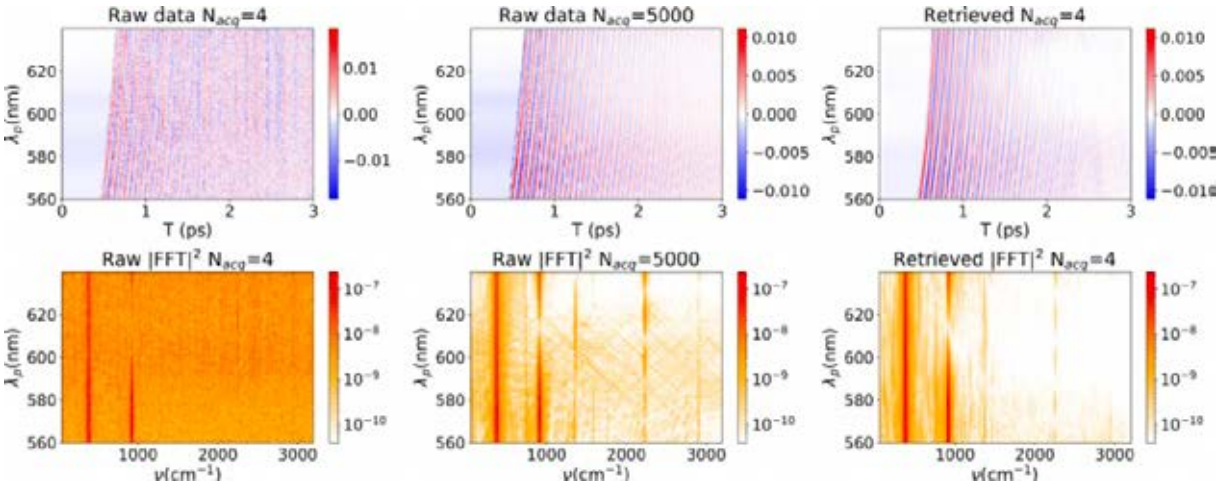
Department of Physics, Sapienza University of Rome, Rome, Italy

Time-domain Impulsive Vibrational Spectroscopy (IVS) and frequency-domain techniques like Stimulated Raman Scattering (SRS) are powerful tools for capturing molecular dynamics. However, broadband detection is fundamentally limited by the readout speed of CCD-based spectrometers, which constrain the operation to the 1–100 kHz regime for single shot detection. Operating within this low-frequency bandwidth presents a severe physical bottleneck: overwhelming $1/f$ laser intensity noise. Consequently, both methodologies heavily dominated by laser fluctuations. Furthermore, IVS faces the intrinsic mathematical vulnerability of the Fast Fourier Transform (FFT), where phase/amplitude noise and truncated acquisition windows are directly converted into spectral broadening, background, artifacts, and leakage.

Here we address the typical broadband IVS scheme, demonstrating a key advantage brought about by chromatic dispersion (namely, a chirp [J. Phys. Chem. Lett. 2024, 15, 25, 6634]) for artificial intelligence (AI)-based denoising. As different probe wavelengths arrive at different times, the vibrational oscillations follow a specific slanted path on the wavelength-delay map (Figure 1). Conversely, noise and laser fluctuations typically manifest as artifacts at specific delays across the entire spectrum. This "geometric" decorrelation provides a unique fingerprint that allows for the effective identification and isolation of genuine signals from the noise. To exploit these features, we introduce a data-driven approach leveraging AI as a highly efficient denoiser for time-domain nonlinear vibrational spectroscopy. By recognizing that genuine vibrational signals and noise exhibit different spectral-temporal correlations across the recorded experimental maps, we have trained specialized neural networks to disentangle them. Our protocol uses residual learning to isolate nonlinear optical signals from complex backgrounds with unprecedented accuracy. The network outperforms standard analysis, suppressing >90% of noise-driven false positives and revealing vibrational modes—in both ground and excited states—that would otherwise remain inaccessible. In Figures 1-2, we demonstrate the algorithm on the experimental spectrum of acetonitrile, showing how the AI-retrieved result from minimal scans matches the quality of classical approaches requiring significantly higher data averages.

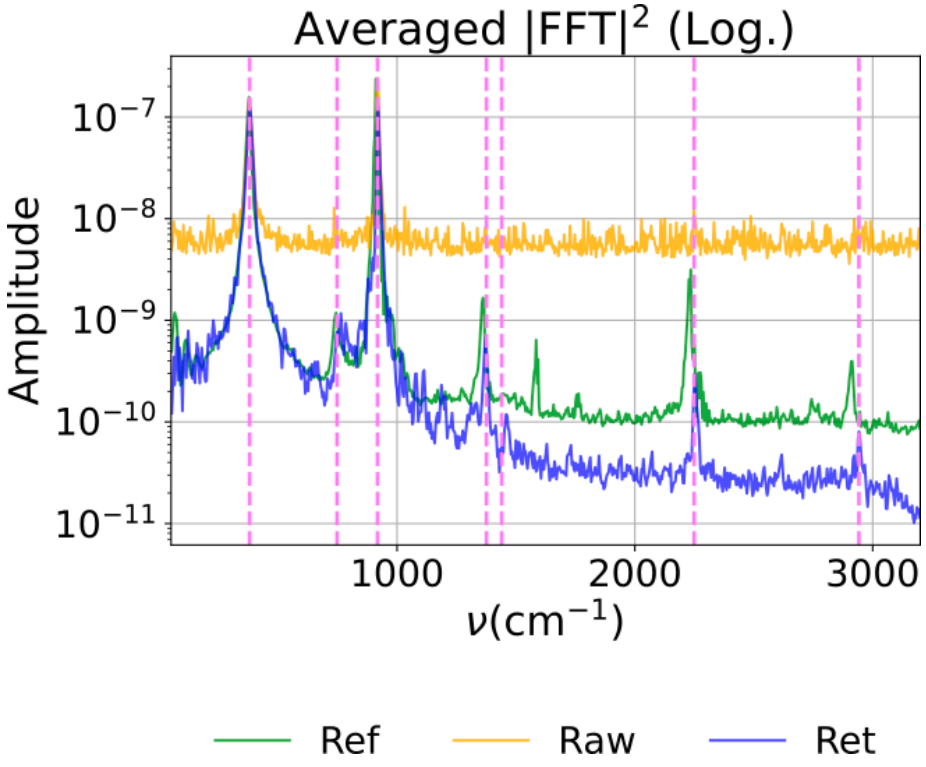
Keywords: Artificial Intelligence, Impulsive Vibrational Spectroscopy, Deep Learning, Data Denoising, Time-Domain Spectroscopy

Figure 1



Experimental data acquired on a sample of acetonitrile using an off-resonant pump and probe. The classical analysis with a number of acquisitions equals 4 (central panels, first and second rows) is compared with the corresponding AI-based reconstruction (right panels, first and second rows) and a measurement with a number of acquisitions equals 5000 used as ground truth (left panels, first and second rows).

Figure 2



Average of the acetonitrile power spectrum (shown in Figure 1) over all probe wavelengths, displayed on a logarithmic scale. Vertical lines indicate the expected spectral peaks reported in the literature.

[Abstract:0405] [Novel Approaches]

Automated Single-nanoparticle Raman: Expanding Possibilities Through Increased Data Volume

***Mathias Novik Jensen*, Nicholas Brækken Nisbet, Noah Horne, Yasser Ben Khalifa, Olav Gaute Hellesø**

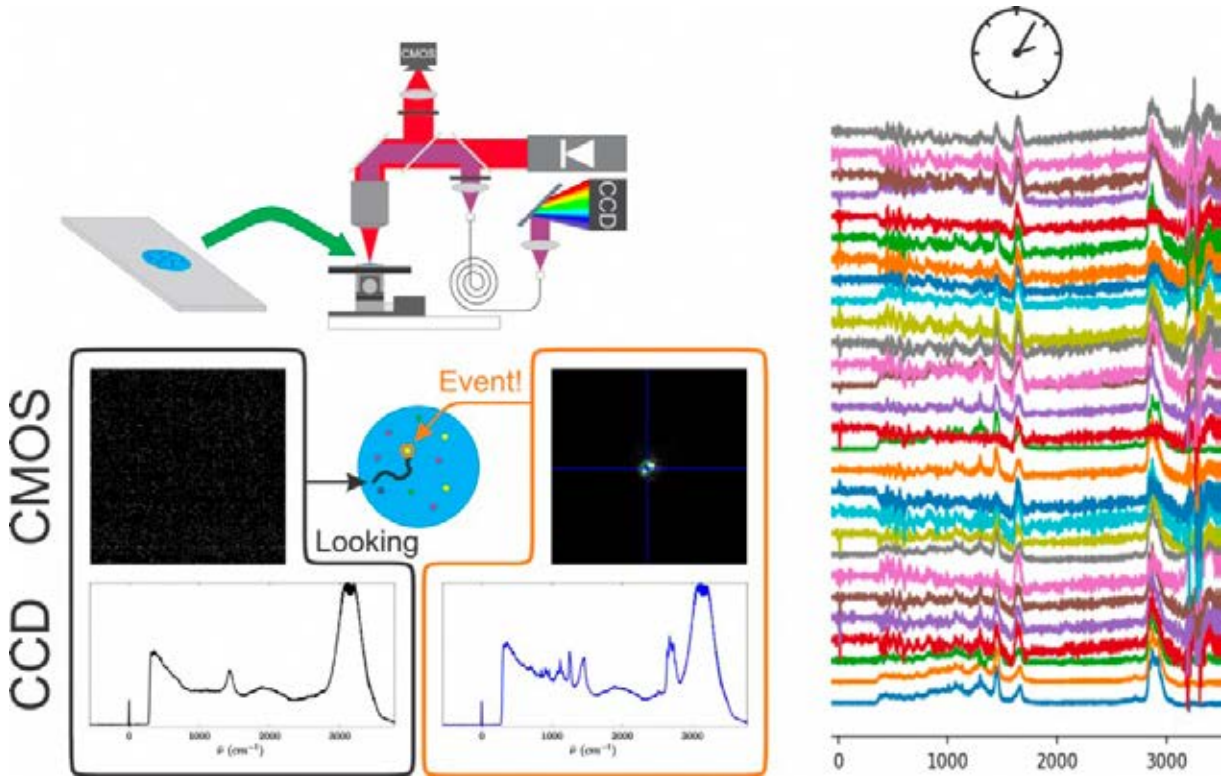
Department of Physics and Technology, UiT The Arctic University of Norway, Tromsø, Norway

One of the unique advantages offered by Raman spectroscopy is the measurement of extremely small discrete volumes, which in combination with optical trapping enables the measurement of nanoparticles on a per-particle basis. This enables the study of a population of nanoparticles, such as extracellular vesicles (EVs), while gathering information about the distribution and heterogeneity of the population. A major challenge in such work is the volume of data required to form an accurate statistical representation of the population, which for nanoparticles can require several thousand individual measurements. Given the difficulty in optically trapping particles significantly smaller than 1um and the correspondingly weak signal, established techniques require the full time of a skilled operator and even then, struggle to get more than 50 trapping events in a day, making it unrealistic to collect the desired volume of data.

We introduce an augmented measurement technique, using automated protocols to both accelerate, standardize and reduce the workload of gathering such volumes. This technique uses a combination of spatial imaging and machine vision together with spectral sensing to detect trapping of micro/nanoparticles, allowing the method to intelligently collect data while relying on inexpensive modification to established systems. This allows the system to operate continuously over long periods of time, thus greatly increasing the number of measurements that can be performed. The method is capable of collecting measurements at average rates of 35 events pr. hour, equating to over 800 measurements in a 24-hour period, a factor 40 higher than what is commonly achieved with manual operation, the result of which will be presented. By also collecting spectra of the ambient medium and using automated signal analysis to detect unique signals the method can produce high-quality spectra without a specifically trained human operator, reducing the associated workload and making the method accessible to scientists not specializing in optics or data processing.

Keywords: Extracellular vesicles, Trapping Raman microspectroscopy, Automation

Illustration of the automated nanoparticle Raman system



The figure illustrates the system (left) which uses a CMOS-based camera for spatial imaging and a fiber-coupled CCD-based spectrometer for spectral measurements. The system uses motorized stages to navigate the sample until the image of scattered light from a trapped nanoparticle is detected and confirmed using its Raman spectrum. The system can measure multiple unique events in a short period of time (right) as demonstrated by the displayed measurements of HEP-1 derived EVs taken by the automated system in 45 minutes.

[Abstract:0407] [Materials]

Decoupling Temperature and Stress in Transferred Silicon Nanomembranes on Heterogeneous Substrates for Elevated-Temperature Applications via Micro-Raman Spectroscopy

***Dooyoung Kim*[1], *Taeyeong Kim*[2], *Doohong Min*[2], *Jungchul Lee*[2]**

[1]*Department of Electrical Engineering, Korea Advanced Institute of Science and Technology, Daejeon, Republic of Korea*
[2]*Department of Mechanical Engineering, Korea Advanced Institute of Science and Technology, Daejeon, Republic of Korea*

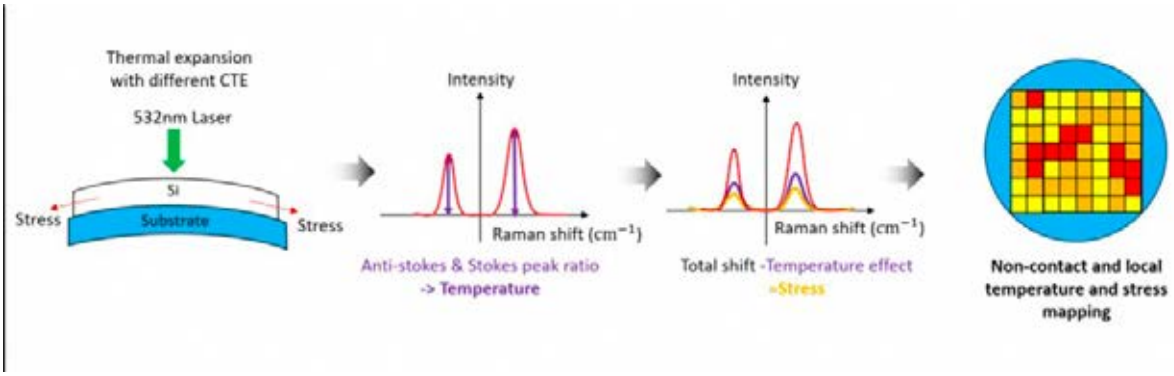
High-temperature annealing can induce curvature-driven morphological transformations in pre-patterned silicon microstructures, enabling unconventional fabrication pathways. In this process, silicon pillars evolve into near-spherical geometries, merge with neighboring structures, and ultimately undergo pinch-off to form continuous silicon nanomembranes. This deterministic, adhesion-free transfer method enables integration of high-quality crystalline silicon onto heterogeneous substrates such as quartz and silicon carbide (SiC), which are otherwise incompatible with conventional bonding or epitaxy.

For applications at elevated temperatures, the transferred nanomembranes experience thermo-mechanical stress due to the mismatch in coefficients of thermal expansion (CTE) between silicon and the underlying substrates. Because temperature and stress effects are inherently coupled in most experimental observables, it remains challenging to quantitatively separate their individual contributions. To address this, we present a micro-Raman spectroscopy–based framework that decouples temperature and stress under controlled thermal loading. The local temperature is extracted from the anti-Stokes to Stokes intensity ratio, while the stress is determined from the Raman peak shift after removing the temperature-dependent contribution using calibrated coefficients.

We apply this approach to silicon nanomembranes transferred onto quartz and SiC substrates, revealing distinct substrate-dependent stress evolution governed by thermal mismatch. The experimentally obtained stress–temperature relationships show strong agreement with thermo-mechanical modeling. This work provides a non-contact, spatially resolved diagnostic platform for heterogeneous systems and offers critical insights for designing reliable silicon-based devices operating under elevated-temperature conditions.

Keywords: Raman, Heterogeneous Substrates, Stress

Figure1



Independent temperature and stress mapping via micro-Raman spectroscopy

[Abstract:0410] [SERS/TERS/Plasmonics]

Controlled Synthesis of Plasmonic Gold Nanostructures for Reproducible SERS Substrates in Biomedical Applications

***Ciprian-Paul Măirean*[1], Septila Renata[1], Dragoș-Ioan Olariu[2], Magdalena Aflori[3], Brindusa Dragoi[4], Rares Stiufiuc[5]**

[1]*Nanotechnology Laboratory, TRANSCEND Research Center, Regional Institute of Oncology, 2-4 General Henri Mathias Berthelot Street, 700483 Iasi, Romania*
[2]*Nanotechnology Laboratory, TRANSCEND Research Center, Regional Institute of Oncology, 2-4 General Henri Mathias Berthelot Street, 700483 Iasi, Romania; Department of Physics of Polymers and Polymeric Materials, "Petru Poni" Institute of Macromolecular Chemistry, 700487 Iasi, Romania*
[3]*Department of Physics of Polymers and Polymeric Materials, "Petru Poni" Institute of Macromolecular Chemistry, 700487 Iasi, Romania*
[4]*Nanotechnology Laboratory, TRANSCEND Research Center, Regional Institute of Oncology, 2-4 General Henri Mathias Berthelot Street, 700483 Iasi, Romania; Faculty of Chemistry, Alexandru Ioan Cuza University of Iasi, 11 Carol I Boulevard, 700506 Iasi, Romania*
[5]*Nanotechnology Laboratory, TRANSCEND Research Center, Regional Institute of Oncology, 2-4 General Henri Mathias Berthelot Street, 700483 Iasi, Romania;Department of Nanobiophysics, MedFuture Research Center for Advanced Medicine, "Iuliu Hațieganu" University of Medicine and Pharmacy, 4-6 Pasteur Street, 400337 Cluj-Napoca, Romania*

Cancer remains one of the leading causes of mortality worldwide, underscoring the urgent need for reliable early diagnostic strategies. Raman spectroscopy, particularly Surface-Enhanced Raman Scattering (SERS), has emerged as a highly sensitive analytical technique enabling the detection of molecular fingerprints at extremely low concentrations. However, its clinical translation remains hindered by the difficulty of fabricating reproducible plasmonic substrates capable of generating stable Raman responses in complex biological fluids.

Plasmonic nanostructures are essential for Raman signal enhancement via localized surface plasmon resonance. Gold nanoparticles are particularly well-suited for biomedical Raman applications due to their chemical stability, tunable optical properties, and high biocompatibility. In this study, spherical and rod-shaped gold nanostructures were synthesized and structurally characterized to develop reproducible SERS substrates for the detection of biomolecular signatures. Gold nanospheres and nanorods were synthesized using a seed-mediated growth approach, allowing precise control over nanoparticle size, morphology, and aspect ratio. The synthesis parameters and purification procedures were optimized to obtain stable colloidal suspensions suitable for SERS investigations in biological environments. The synthesized nanostructures were characterized using complementary analytical techniques (UV-vis spectroscopy, Dynamic Light Scattering, Zeta potential, and Transmission Electron Microscopy).

The synthesized nanostructures exhibited excellent colloidal stability for more than 30 days without aggregation or significant spectral shifts. Preliminary SERS measurements performed on here-presented plasmonic substrates using several Raman active probe molecules demonstrated strong and reproducible signal enhancement. Furthermore, SERS analyses of biological samples, including serum collected from oncological patients, indicate the potential of the developed substrates for detecting molecular signatures relevant to biomedical diagnostics.

These findings indicate that precise control over nanoparticle synthesis and stabilization is essential for generating reproducible SERS substrates, while underscoring the potential of engineered plasmonic nanostructures in biomedical Raman sensing and point-of-care diagnostics.

Keywords: plasmonic nanoparticles, Raman spectroscopy, SERS, biomedical diagnostics

[Abstract:0418] [Materials]

A Microfluidic SERS Platform for Real-time Monitoring of Antiepileptic Drugs

***Lydia Federica Gervasini*[1], *Annachiara D'urso*[2], *Emilio Ciusani*[2], *Alessia Cutri*[1], *Sebastiano Trusso*[3], *Paolo Maria Ossi*[4], *Andrea Lucotti*[1], *Nisha Rani Agarwal*[5], *Matteo Tommasini*[1]**

[1]*Dipartimento di Chimica, Materiali e Ingegneria Chimica "G. Natta", Politecnico di Milano, 20133 Milano, Italy*
[2]*Laboratorio di Patologia Clinica e Genetica Medica, Fondazione IRCCS Istituto Neurologico Carlo Besta, Via Celoria 11, 20133 Milano, Italy*
[3]*Istituto per i Processi Chimico-Fisici (IPCF), CNR, 98158 Messina, Italy*
[4]*Dipartimento di Energia, Politecnico di Milano, 20133 Milano, Italy*
[5]*Nano-Imaging and Spectroscopy Laboratory, Faculty of Science, Ontario Tech University, Oshawa, Canada*

Therapeutic drug monitoring (TDM) of antiepileptic drugs (AEDs) is essential for effective seizure control due to their narrow therapeutic index (NTI), high interpatient variability, and complex pharmacokinetics. However, conventional analytical techniques such as HPLC and LC–MS are time-consuming, require specialized infrastructure, and are not well-suited for rapid or point-of-care applications.

To address these limitations, we propose a microfluidic analytical platform integrating surface-enhanced Raman spectroscopy (SERS) with embedded plasmonic gold nanoparticles (AuNPs) for sensitive, label-free, and low-volume detection of clinically relevant AEDs. The platform is based on a laser-etched polydimethylsiloxane (PDMS) microchannel (5 μL) incorporating SERS-active AuNP substrates synthesized via the controlled Turkevich citrate reduction method. This architecture is designed to enable real-time chemical fingerprinting under continuous or semi-continuous flow conditions while maintaining high surface enhancement and reproducibility.

Representative AED samples are introduced into the microfluidic channel to explore the acquisition of reproducible SERS spectra across clinically relevant concentration ranges. The system is being evaluated for its ability to provide reliable spectral identification and to operate in the presence of potential matrix interferences arising from biological fluids or pharmaceutical excipients.

The proposed microfluidic–SERS platform represents a promising approach for rapid pharmaceutical analysis and may provide the basis for the development of compact diagnostic tools for personalized antiepileptic therapy. Ongoing work is focused on assessing analytical performance and investigating drug–matrix and drug–nanoparticle interactions.

Keywords: SERS, gold nanoparticles, microfluidics, epilepsy, therapeutic drug monitoring

[Abstract:0436] [Industrial/Societal Applications]

Determination of Methanol in Alcoholic Beverages by Raman Spectroscopy: The Effect of Using Different Internal Standards on Method Performance

***Kübra Güven*[1], *Akif Goktug Bozkurt*[2], *Ismail Hakki Boyaci*[1], *Ugur Tamer*[3]**

[1]*Department of Food Engineering, Hacettepe University, Ankara, Türkiye*
[2]*Department of Food Processing, Vocational School of Technical Sciences, Ardahan University, Ardahan, Türkiye*
[3]*Department of Analytical Chemistry, Faculty of Pharmacy, Gazi University, Ankara, Türkiye*

Methanol in alcoholic beverages poses a serious health risk; even a low concentration of 300–1000 mg/kg can cause metabolic acidosis, optic neuropathy and death. The legal methanol detection limit for distilled alcoholic beverages is 0.087 M for 40% alcohol by volume. Raman spectroscopy offers a non-reactive, non-destructive and rapid alternative. In previous studies, methanol has generally been determined using an acetonitrile internal standard with detection limits ranging from 0.99 to 4.25 mM. In the ethanol–methanol–water matrix, a standard prone to hydrogen bonding causes peak shifts that distort linearity, making the choice of internal standard critical. In this study, five internal standards (IS) with different polarities (acetonitrile, propanol, ethyl acetate, acetone and 1-butanol) were evaluated with the aim of minimising the limit of detection (LOD) and the limit of quantification (LOQ) for methanol in commercial alcoholic beverages.

Measurements were performed using 400 µL liquid samples with a 20 second integration time. In the calibration solutions, the methanol concentration (0.25–5% v/v) was varied whilst the ethanol concentration (40% v/v) and each internal standard (10% v/v) were kept constant. Six commercial alcoholic beverages were analysed.

Acetonitrile and ethyl acetate yielded the highest calibration linearity ($R^2 > 0.98$). Acetone, propanol, and 1-butanol performed markedly worse ($R^2 < 0.87$). The superior performance of acetonitrile is attributed to its chemical inertness, spectral isolation of its C≡N stretching band (~918 cm^{-1}), and low susceptibility to hydrogen-bonding perturbations in the ternary matrix. Inferior IS candidates engaged in competitive hydrogen-bonding with matrix components, inducing systematic shifts in both their Raman bands and the methanol analytical peak.

As a result of using acetonitrile as the standard in six different commercial alcoholic beverages, R^2 values of 0.9804–0.9954, LOD of 0.308–0.378%, LOQ of 0.933–1.145% (w/w) were obtained. Consistent linearity across vodkas, gins, and raki confirms method robustness. Notably, fixed-concentration IS and ethanol bands shifted as methanol varied, reflecting co-solvent-driven changes in bulk dielectric constant and polarisability of the ethanol–methanol–water system. This mechanistically explains IS-dependent performance differences and highlights the importance of selecting a matrix-insensitive IS for reliable Raman-based methanol quantification in complex alcohol matrices.

Keywords: Raman spectroscopy, methanol detection, internal standard, alcoholic beverages, spectral interference.

[Abstract:0438] [SERS/TERS/Plasmonics]

Electrochemical SERS of Aromatic Thiols on Silver: Potential-Dependent Study of Charge-Transfer and Molecule–Metal Interactions

***Jakub Havránek*[1], *Matěj Kmetík*[1], *Ivan Kopal*[2], *Marcela Dendisová*[3]**

[1]*Department of Physical Chemistry, University of Chemistry and Technology, Prague, Czech Republic, Analytical Laboratory, Institute of Organic Chemistry an Biochemistry of the CAS, Prague, Czech Republic*
[2]*Institute of Photonics and Electronics, Czech Academic of Sciences, Prague, Czech Republic, Department of Physical Chemistry, University of Chemistry and Technology, Prague, Czech Republic*
[3]*Department of Physical Chemistry, University of Chemistry and Technology, Prague, Czech Republic*

Electrochemical surface-enhanced Raman scattering (EC-SERS) enables a detailed probing of molecule–metal interactions at electrified interfaces with high sensitivity and molecular specificity. However, interpretation of potential-dependent SERS spectra remains challenging due to the interplay of electromagnetic and chemical enhancement mechanisms, as well as potential electrochemical transformations of the analyte. The application of an external potential allows for controlled adsorption and enables investigation of charge-transfer processes that contribute to chemical enhancement.

Here, we investigate aromatic thiols, 4-aminobenzenethiol (4-ABT) and p-xylene-α-thiol (ALPHA), adsorbed on a silver substrate. A custom-built spectroelectrochemical cell compatible with a Renishaw inVia Raman microscope allowed in-situ monitoring of adsorption kinetics both under open-circuit conditions and under applied potential (Figure 1, Spectroelectrochemical cell). SERS and EC-SERS measurements were performed using excitation wavelengths of 532, 633, and 785 nm, allowing us to probe wavelength-dependent effects.

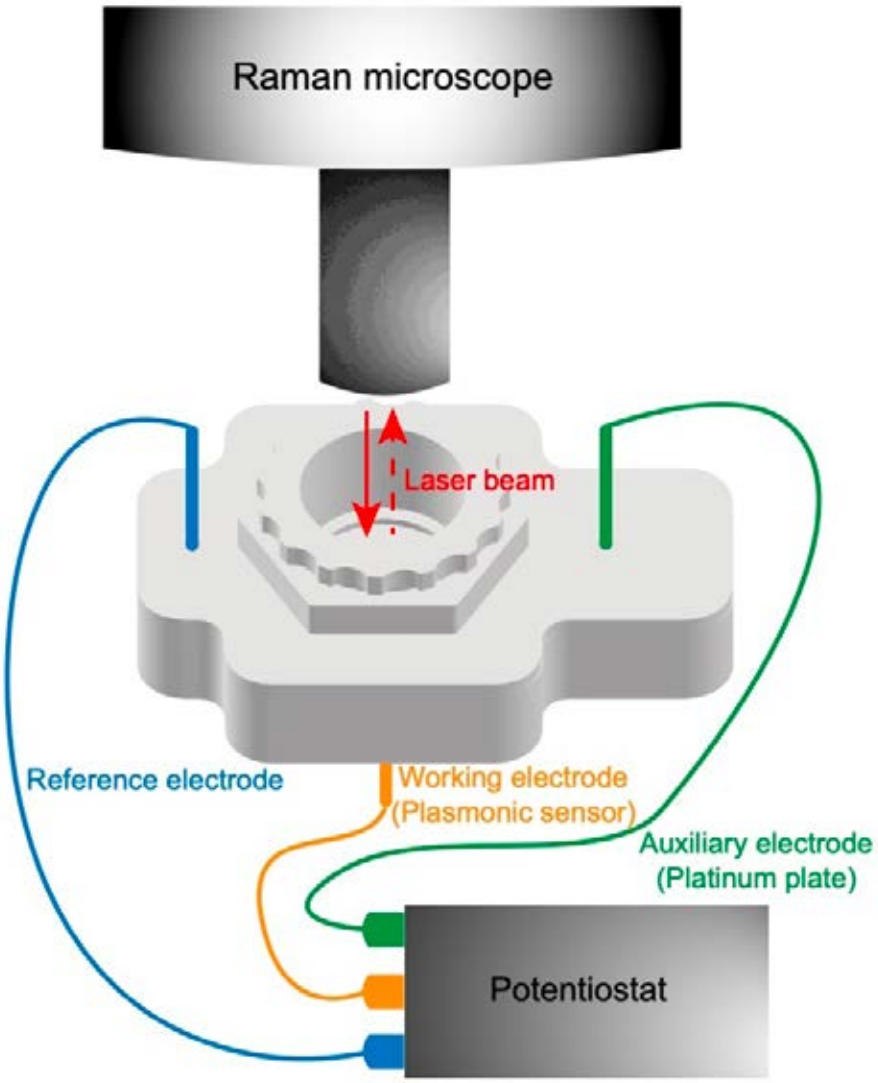
Different enhancement pathways are identified for the studied molecules. In the case of 4-ABT, the observed spectral changes indicate a charge-transfer mechanism involving transitions between the molecular LUMO and the Fermi level of the silver substrate. This interaction depends on both the applied potential and the excitation wavelength. For p-xylene-α-thiol (ALPHA), the results suggest the involvement of additional molecule–metal interactions beyond a simple charge-transfer model, which may contribute to the observed spectral response and adsorption behavior.

The experimental observations are supported by density functional theory (DFT) calculations, which elucidate the electronic structure of the adsorbed species and their interaction with the metal surface. The combined experimental and theoretical approach demonstrates the role of molecule–metal coupling in EC-SERS.

Overall, these results provide a deeper understanding of chemical enhancement mechanisms and interfacial charge-transfer processes in plasmonic systems.

Keywords: EC-SERS, silver substrate, potential, thiols, charge transfer

Figure 1, Spectroelectrochemical cell



[Abstract:0443] [SERS/TERS/Plasmonics]

In situ Synthesis of Silver Nanoparticles for Surface-Enhanced Raman Spectroscopy-Based Detection of Carbendazim Residues on Apple Surfaces

sevda mert

Department of Genetics and Bioengineering, Faculty of Engineering, Istanbul Okan University, Istanbul, Turkey

The rapid detection of pesticide residues on fresh produce remains a critical challenge for food safety monitoring. In this study, an in situ silver nanoparticle (AgNP) synthesis strategy was investigated to enhance surface-enhanced Raman spectroscopy (SERS) signals for the detection of carbendazim residues on apple surfaces. Crystal violet (CV) was employed as a model analyte to systematically optimize synthesis parameters, including the concentrations and addition sequence of $AgNO_3$, hydroxylamine hydrochloride ($HONH_2{\cdot}HCl$), and NaOH. A large number of in situ synthesis protocols were initially screened; however, only four protocols yielded sufficiently strong and reproducible SERS signals and were therefore selected for further investigation. A key finding of this study is the strong dependence of SERS performance on the nanoparticle formation strategy. AgNPs synthesized ex situ and subsequently mixed with the analyte produced weak and poorly defined SERS signals, indicating insufficient hotspot formation. In contrast, in situ synthesis of AgNPs directly within the analyte environment resulted in significantly enhanced spectral intensity, suggesting improved nanoparticle–analyte interactions and more effective hotspot generation. Nevertheless, this approach exhibited lower reproducibility, likely due to variations in nucleation and growth dynamics during nanoparticle formation. Carbendazim residues were applied onto apple surfaces and extracted using methanol. The extracts were subjected to the selected in situ protocols, and SERS spectra were acquired using an 785 nm excitation source over the spectral range of 300–1200 cm^{-1}. Comparative evaluation of the four optimized protocols revealed notable differences in signal enhancement efficiency, emphasizing the critical role of synthesis conditions in SERS performance.

Keywords: Surface-enhanced Raman Spectroscopy, AgNPs, Carbendazim, in situ synthesis

Posters

[Abstract:0444] [SERS/TERS/Plasmonics]

Soft Actuator-Based Reconfigurable Platforms for SERS

***Görkem Liman*[1], *Hayrettin Öner*[2], *Gökhan Demirel*[1]**

[1]*Bio-inspired Materials Research Laboratory (BIMREL), Department of Chemistry, Gazi University, 06500 Ankara, Turkey*
[2]*Gazi University Institute of Science, Department of Chemistry, Gazi University, 06500 Ankara, Turkey*

Surface-enhanced Raman spectroscopy (SERS) has emerged as a highly sensitive analytical technique capable of detecting molecular species at ultralow concentrations. Despite its remarkable sensitivity, conventional SERS platforms still face critical limitations in controllable hot-spot generation, scalability, and adaptability to complex surfaces. Recent advances in soft materials and stimuli-responsive systems offer new opportunities to overcome these challenges.

In this study, we present a soft actuator-based SERS platform that enables dynamic, controllable manipulation of plasmonic hot-spot formation via polymer deformation. Unlike traditional rigid substrates, the proposed system uses stimuli-responsive polymeric structures that can reversibly fold and reconfigure. This structural adaptability allows precise tuning of interparticle distances, directly influencing localized surface plasmon resonance and Raman signal enhancement. The platforms also support effective sample collection and transport through externally controlled motion, enhancing interaction between analyte molecules and active sensing regions. Such dynamic behavior is particularly advantageous for detecting analytes on non-planar or irregular surfaces, where conventional rigid substrates fail to achieve sufficient contact

Raman spectroscopy is employed not only as a detection tool but also as an in-situ characterization method to monitor structural and chemical changes within the actuator system. This dual functionality highlights the synergy between soft actuation and spectroscopic analysis. The results demonstrate that soft-actuator-integrated SERS systems provide a versatile, scalable approach for next-generation sensing technologies.

Acknowledgments: This work was supported by the Scientific and Technological Research Council of Türkiye (TUBITAK) (grant no: 22AG056).

Keywords: Raman Spectroscopy, SERS, Hot Spot Engineering, Soft Actuator

Posters

[Abstract:0445] [SERS/TERS/Plasmonics]

Impact of Data Partitioning Strategies on SERS-Based Machine Learning for Reliable Classification of Antibiotic Resistance in Staphylococcus aureus

***Zakarya Al Shaebi*[1], *Munevver Akdeniz*[1], *Serra Ilayda Yerlitas Tastan*[2], *Pınar Sagiroğlu*[3], *Mustafa Altay Atalay*[3], *Gözde Ertürk Zararsiz*[2], *Gökmen Zararsiz*[4], *Omer Aydin*[5]**

[1]Department of Biomedical Engineering, Erciyes University, Kayseri, 38039, Türkiye, NanoThera Lab, ERFARMA-Drug Application and Research Center, Erciyes University, Kayseri, 38280, Türkiye
[2]Department of Biostatistics, School of Medicine, Erciyes University, Kayseri, Türkiye
[3]Department of Medical Microbiology, Faculty of Medicine, Erciyes University, 38039, Kayseri, Türkiye
[4]Department of Biostatistics, Erciyes University School of Medicine, Kayseri, Türkiye. Hematainer Biotechnology and Health Products Inc., Erciyes Teknopark, 38039, Kayseri, Türkiye
[5]Department of Biomedical Engineering, Erciyes University, Kayseri, 38039, Türkiye. NanoThera Lab, ERFARMA-Drug Application and Research Center, Erciyes University, Kayseri, 38280, Türkiye. ERNAM-Nanotechnology Research and Application Center, Erciyes University, Kayseri, 38039, Türkiye. ERKAM-Clinical Engineering Research and Implementation Center, Erciyes University, Kayseri, 38030, Türkiye. Drug Application and Research Center (ERFARMA), Erciyes University, Kayseri, Türkiye. Betül-Ziya Eren Genome and Stem Cell Center, Erciyes University, Kayseri, Türkiye

Antimicrobial resistance (AMR) remains a critical global health challenge, demanding rapid and reliable diagnostic approaches. Surface-enhanced Raman spectroscopy (SERS) has emerged as a powerful tool for capturing biochemical fingerprints of microorganisms, while machine learning (ML) enables automated interpretation of complex spectral data. However, the reliability of SERS–ML systems is strongly influenced by data handling strategies, which are often overlooked. In this study, we investigated the effect of different data partitioning approaches on the performance and generalizability of SERS-based ML models for classifying Staphylococcus aureus isolates. SERS spectra were collected from methicillin-resistant (MRSA), erythromycin-resistant (ERSA), and antibiotic-sensitive (SSA) strains using silver nanoparticle enhancement, generating a large spectral dataset across multiple isolates. Preprocessing included baseline correction, smoothing, and normalization, followed by feature selection using Boruta and LASSO, and dimensionality reduction via principal component analysis (PCA). Five machine learning algorithms-k-nearest neighbors, random forest, support vector machine, neural networks, and extreme gradient boosting-were systematically evaluated under multiple data partitioning scenarios, including spectrum-level, sample-level, and isolate-level splitting. The results revealed that models trained and tested on non-independent spectra produced artificially high performance, whereas isolate-level partitioning provided a more realistic estimation of model generalizability, albeit with reduced accuracy. Among the tested approaches, random forest combined with Boruta feature selection demonstrated the most consistent and interpretable performance across scenarios. The findings highlight that data partitioning strategy is a critical determinant of reported model accuracy in SERS-based diagnostics. This work emphasizes the need for standardized evaluation frameworks in SERS–ML studies and provides practical guidelines for developing robust, clinically translatable Raman-based diagnostic systems for antimicrobial resistance detection.

This work has been supported by Erciyes University Scientific Research Projects Coordination Unit under grant number # FBAÜ-2023-12265.

Keywords: SERS, AMR, Staphylococcus aureus, Machine Learning, Data Partitioning

Posters

[Abstract:0446] [SERS/TERS/Plasmonics]

SERS-Based Spectral Fingerprinting of Brucella in Body Fluids Coupled with Machine Learning

***Munevver Akdeniz*[1], *Zakarya Al Shaebi*[1], *Fatma Mutlu Sarıgüzel*[2], *Pınar Sagiroglu*[2], *Mustafa Altay Atalay*[2], *Omer Aydin*[3]**

[1]*Department of Biomedical Engineering, Erciyes University, Kayseri, 38039, Türkiye, NanoThera Lab, ERFARMA-Drug Application and Research Center, Erciyes University, Kayseri, 38280, Türkiye*
[2]*Department of Medical Microbiology, Faculty of Medicine, Erciyes University, 38039, Kayseri, Türkiye*
[3]*Department of Biomedical Engineering, Erciyes University, Kayseri, 38039, Türkiye, NanoThera Lab, ERFARMA-Drug Application and Research Center, Erciyes University, Kayseri, 38280, Türkiye, ERNAM-Nanotechnology Research and Application Center, Erciyes University, Kayseri, 38039, Türkiye, ERKAM-Clinical Engineering Research and Implementation Center, Erciyes University, Kayseri, 38030, Türkiye, Betül-Ziya Eren Genome and Stem Cell Center, Erciyes University, Kayseri, Türkiye*

Brucellosis is a zoonotic disease caused by Brucella spp., a gram-negative bacterium, posing significant risks to human and animal health and causing substantial economic losses. Accurate and rapid detection of Brucella is critical to prevent transmission. Conventional diagnostic methods, including bacterial culture, serological assays, and PCR-based techniques, are limited by high cost, long processing times, and the need for specialized personnel and biosafety facilities. Therefore, there is a need for rapid and more efficient diagnostic approaches that can also evaluate the impact of infection on bodily fluids. Surface-Enhanced Raman Spectroscopy (SERS) enhances Raman signals of molecules adsorbed onto nanostructured metallic surfaces and has emerged as a promising technique for rapid bacterial infection of biological fluids. When combined with machine learning, SERS data can be effectively processed for accurate sample classification. In this study, we investigated molecular changes in serum and cerebrospinal fluid (CSF) associated with Brucella infection. Serum samples were divided into negative (1/20, 1/40, 1/80), positive (1/160, 1/320, 1/640, 1/5120), and control groups to reflect clinically relevant antibody titers. SERS spectra were obtained using silver nanoparticles (AgNPs) from serum and CSF samples, and machine learning algorithms, including Random Forest, Support Vector Machine, k-nearest neighbor, Logistic Regression, and Decision Tree, were applied to differentiate the groups. The models achieved 98% accuracy, revealing clear spectral differences between infected and healthy samples. These findings highlight the strong potential of integrating SERS with machine learning as a rapid, sensitive, and reliable approach for detecting bacterial infections in biological fluids, offering promising applications in clinical diagnostics.

Keywords: Brucella spp., Brucellosis, Surface-Enhanced Raman Spectroscopy, Machine learning

Posters

[Abstract:0451] [SERS/TERS/Plasmonics]

Cost-Effective SERS Platforms Based on AuNP-Functionalized Carbonized Polyimide for Fluorescence-Suppressed Raman Detection

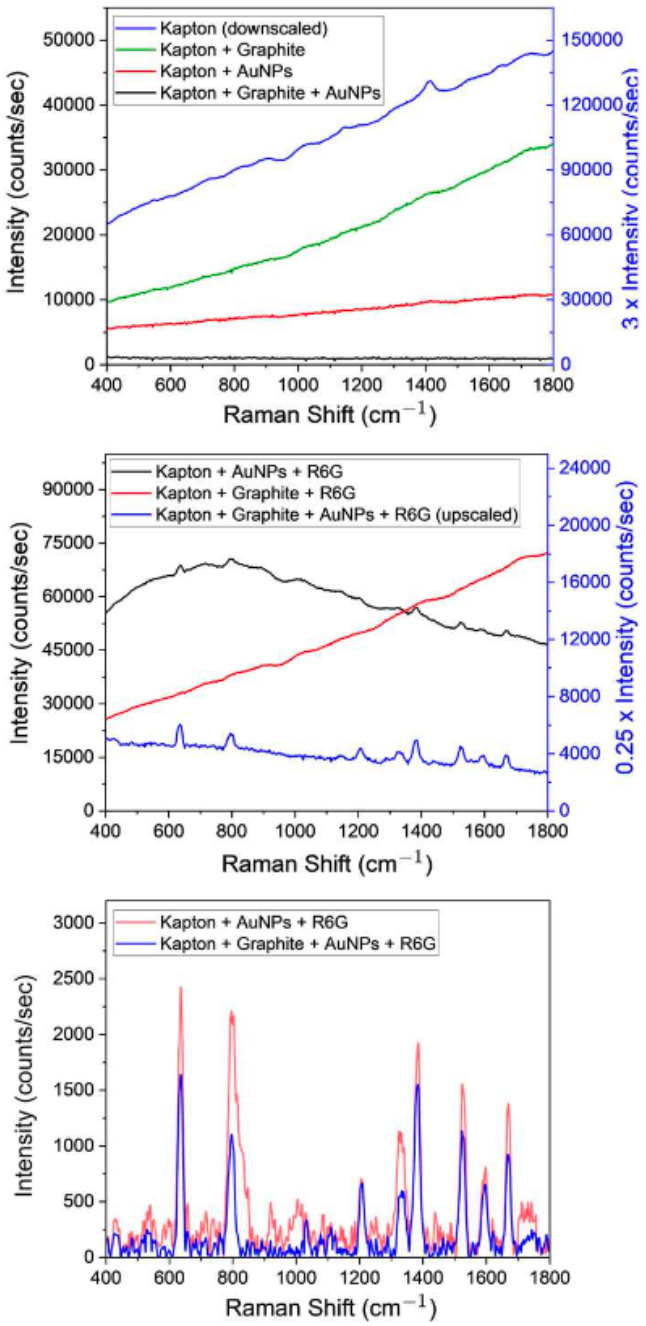
***Sinan GENC*[1], *Ghazanfar Ali Khan*[2], *Dogac Tuzel*[2], *Sumeyye Kina*[3], *Alpan Bek*[3], *Kamil CINAR*[2]**

[1]*Department of Electrical Electronics Engineering, Abdullah Gül University, Kayseri, Turkey*
[2]*Department of Physics, Middle East Technical University, Ankara, Turkey*
[3]*Department of Physics, Gebze Technical University, Kocaeli, Turkey*

Surface-enhanced Raman spectroscopy (SERS) is widely employed for sensitive molecular detection; however, its performance is often limited by strong fluorescence backgrounds, particularly for highly emissive analytes. In this study, a low-cost and scalable hybrid SERS platform is developed by integrating laser-carbonized polyimide films with colloidally synthesized gold nanoparticles (AuNPs). The carbonized polyimide provides a graphitic surface that effectively suppresses fluorescence via charge and energy transfer mechanisms, while the AuNPs introduce localized surface plasmon resonances for Raman signal amplification. Rhodamine 6G (R6G) is used as a model analyte to systematically evaluate the interplay between enhancement and background suppression across multiple substrate configurations. The combined AuNP-decorated graphitized polyimide substrate demonstrates a significant improvement in signal-to-noise ratio, achieving clear Raman peak resolution with strongly reduced fluorescence compared to pristine or single-component counterparts. Quantitative analysis indicates that while graphitic substrates alone suppress both fluorescence and Raman intensity, their integration with AuNPs yields a synergistic effect, enhancing Raman signals while maintaining low background noise. The fabrication process relies on simple laser carbonization and drop-casting techniques, ensuring reproducibility and scalability without requiring complex nanofabrication steps. These results highlight the potential of carbon–plasmonic hybrid substrates as practical, cost-effective solutions for in-situ Raman sensing of fluorescent species in real-world applications.

Keywords: SERS, Raman, fluorescence, polyamide

Figure 1



Comparison of (a) bare Raman spectra in absence of analyte, (b) Raman spectra of R6G on different substrates, and (c) baseline corrected Raman spectra of R6G on bare/graphitized polyimide tape with AuNPs.

[Abstract:0460] [SERS/TERS/Plasmonics]

Copper Oxide Nanostructures for UV- SERS

***Gytaute Sirgedaite*[1], *Martynas Talaikis*[1], *Gediminas Niaura*[1], *Vladimir Sivakov*[2], *Shivani Yadav*[2], *Lina Mikoliunaite*[1]**

[1]*Department Of Organic Chemistry, Center For Physical Sciences And Technology (FTMC), Vilnius, Lithuania*
[2]*Spectroscopy and Imaging, Leibniz Institute of Photonic Technology, Jena, Germany*

Surface-enhanced Raman scattering (SERS), first reported in 1974 by Fleischmann, is a highly sensitive, nondestructive analytical technique for detecting chemical compounds and biomolecules with excellent reproducibility. Conventional SERS applications typically operate in visible to near-infrared spectral range, where strong Raman signal enhancement is achieved However, extension of SERS into ultraviolet (UV) region (UV-SERS) offers significant advantages, particularly for molecules exhibiting strong UV absorption.

Many organic and biological molecules, including nucleic acids (DNA, RNA) and proteins, exhibit electronic transitions in the UV region, enabling resonance Raman enhancement of up to eight orders of magnitude. Despite this potential, traditional SERS substrates based on Au and Ag are not optimal for UV applications due to their high reflectivity and low absorption in this spectral region, limiting electromagnetic field enhancement.

To address these limitations, alternative plasmonic materials such as Al, Pt, Pd, Co, and Cu have been explored. Among these, copper-based nanostructures, particularly cuprous oxide (Cu_2O), are promising candidates due to their ability to provide additional chemical enhancement mechanisms. Recent studies have demonstrated that nanostructured copper films with a preserved Cu_2O layer significantly enhance UV-SERS signals via charge-transfer interactions at the Cu_2O - molecule interface, highlighting the potential of Cu_2O nanoparticle-based composites as effective substrates.

In this work, Cu_2O nanoparticles (NPs) were synthesized using a reduction method and characterized by X-ray diffraction, scanning electron microscopy, dynamic light scattering, and Raman spectroscopy. Furthermore, Cu_2O NPs were combined with magnetic nanoparticles to form composite structures. Both Cu_2O and magnetic-Cu_2O composites were evaluated as substrates for UV-SERS measurements using adenine as UV range-active probe molecule. SERS spectra of adenine were recorded using excitation wavelengths of 325 nm, 442 nm, and 532 nm to assess the enhancement performance.

Keywords: Copper Oxide nanoparticles, UV-SERS, ultraviolet, SERS.

[Abstract:0468] [Novel Approaches]

A New Strategy For On-Site Determination of Phosphorylated Tyrosine Using Modified Lateral Flow Immunoassay Coupled with Surface-Enhanced Raman Spectroscopy

***Jianfeng Wu*, Yichun Chen, Nannan Li, Yulong Liu, Kuo Qi, Jianwei Xie**

Laboratory of Toxicant Analysis, Academy of Military Medical Sciences, Beijing, China

BACKGROUND: Organophosphorus nerve agents (OPNAs) pose severe threats to human health and public safety by damaging the central nervous system through the inhibition of acetylcholinesterase (AChE) activity. The rapid and reliable identification of OPNAs exposure is crucial for safety protection and effective medical treatment. Phosphorylated tyrosine serves as an important long-lived biomarker for identifying exposure to OPNAs. However, the rapid on-site determination of phosphorylated tyrosine remains challenging due to its low concentration and the long digestion time required.

EXPERIMENTS: In this work, a packed-bed immobilized enzyme microreactor was developed using γFe_2O_3 magnetic microspheres activated by NHS-EDC for the immobilization of αchymotrypsin. This microreactor achieved rapid enzymatic hydrolysis to generate phosphorylated tyrosine (Figure. 1a). Subsequently, monoclonal antibodies specifically recognizing OPNA-Tyr were screened using antigens prepared by conjugating phosphorylated tyrosine with Keyhole Limpet Hemocyanin (KLH). Three monoclonal antibodies (coded as mc-8, mc-10, and mc-3, with GB-Tyr-KLH, GD-Tyr-KLH, and VX-Tyr-KLH as immunogens, respectively) were successfully obtained through animal immunization, serum screening, cell fusion, and monoclonal antibody purification. Additionally, co-modification of Raman reporter molecules and antibodies on the surface of gold nanoparticles (AuNPs) was performed (Figure. 1b).

RESULTS: The results showed that the digestion of OPNAs-exposed human serum albumin (HSA) could be completed within 1 h, which was significantly shorter than that of traditional solution enzymatic hydrolysis. It was found that the half-maximal inhibitory concentrations (IC_{50}) of the antibodies for GD-Tyr, GB-Tyr, and VX-Tyr were approximately 5 ng/mL, 80 ng/mL, and 110 ng/mL, respectively (Figure. 1c, 1d, 1e). Subsequently, lateral flow immunoassay (LFIA) was prepared using AuNPs co-modified with antibody mc-10 and an optimal Raman reporter (Figure. 2a). The results demonstrated that this form of LFIA could not only be coupled with a Raman spectrometer but also the detection limit is reduced by nearly two orders of magnitude (0.5 ng/mL) compared with the naked eye colorimetric identification (50 ng/mL) (Figure. 2b and 2c). The detection limit could meet the needs of real sample confirmation. Furthermore, the whole detection procedure requires no complex sample pretreatment and can be conducted on-site, thus enabling point-of-care testing (POCT) for OPNA exposure (Figure. 2d).

Keywords: Organophosphorus nerve agents, tyrosine adduct, LFIA, monoclonal antibody, SERS

Figure 1. (a) The diagram of packed-bed immobilized enzyme microreactor; (b) Scheme the LFIA using the AuNPs modified by Ab and Raman probe; (c), (d) and (e) ELISA evaluation profile of antibodies for GD-Tyr, GB-Tyr and VX-Tyr, respectively.

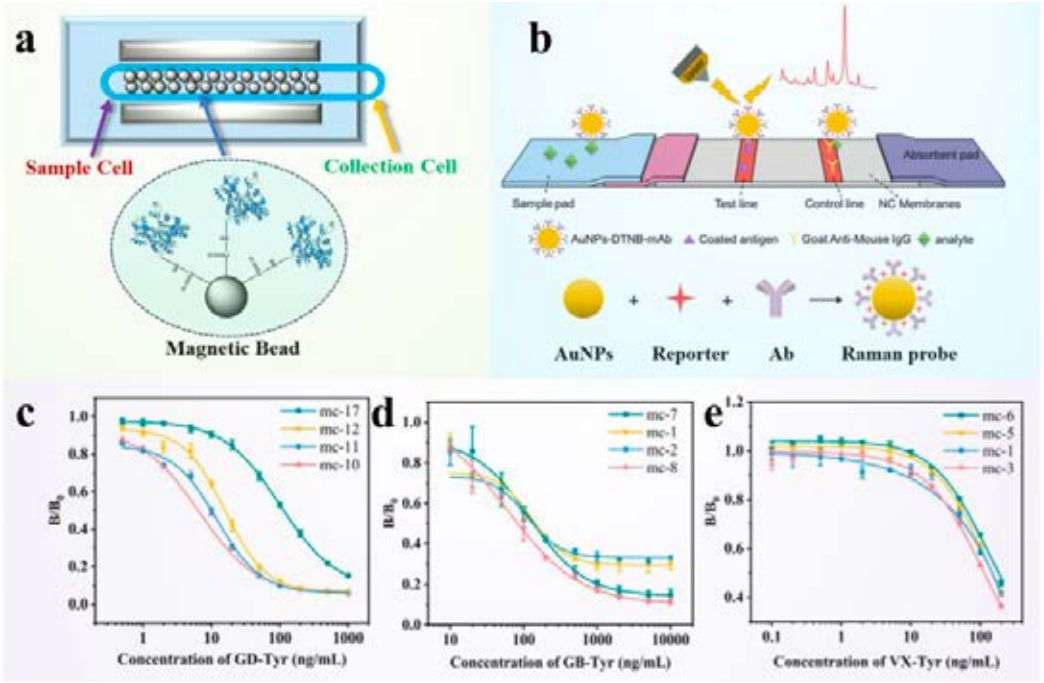
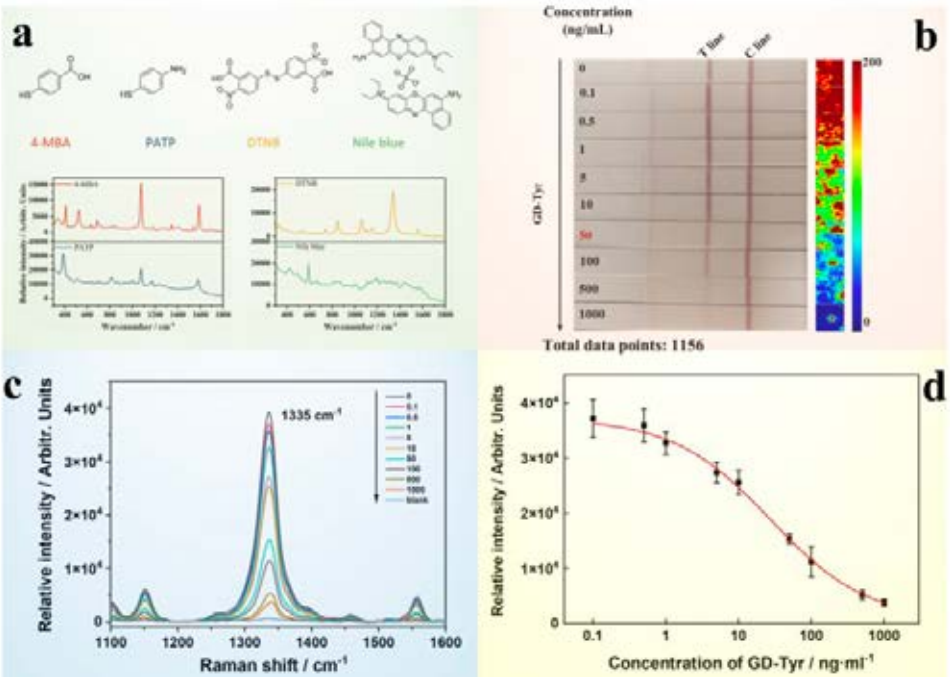


Figure 2. (a) Comparison of different Raman probes; (b) Naked-eye colorimetric detection based on bare colloidal gold LFIA; (c) SERS intensity of probe under different concentration of GD-Tyr; (d) The SERS intensity of Raman signal at 1335cm-1.



[Abstract:0471] [Biology/Biomedicine]

Microplastics Monitoring in Human Breast Milk with Raman Microspectroscopy – A Contamination-Free Sample Collection, Preparation and Measurement Approach

***Felix Thier*, Carla Schachner, Ievgeniia Lomako, Kathrin Gosch, Christina Hartmann, Sebastian Köppel**

Environment Agency Austria (Umweltbundesamt GmbH), Vienna, Austria

Even though awareness about microplastics (MPs) dramatically increased over the past years, information on their distribution in the human body and possible adverse effects on our health is still scarce. Recent studies indicate that human breast milk can act as a potential gateway for MPs. Thus, there is an urgent need for robust methods to characterize these tiny polymer particles in human bodily fluids.

In this work, we present an approach for contamination-free (i.e., plastic-free) sample collection, preparation and measurement to quantify MPs in the size range of 1 – 25 µm with Raman microspectroscopy (µRaman) in human breast milk. Preliminary experiments led to the establishment of a sample preparation protocol based on digestion and filtration steps to selectively separate MP particles from the breast milk matrix. Sample preparation and µRaman measurements on suitable substrates were carried out under controlled laboratory conditions. This enabled the development of an optical particle recognition workflow combined with µRaman for particle identification. A wide range of blank samples (i.e., reagent, equipment, method and field blanks) aided in monitoring the success of contamination-free procedures. Preliminary results show that blank samples contain significantly less MP particles compared to a previously collected human breast milk sample: with respect to the total particle count, the fraction of MP particles was 2.60% in the breast milk sample, in contrast to 0.65% in the method blank sample.

The next step involves the application of the contamination-free sample collection protocol by ten breastfeeding mothers, followed by quantifying the ten most common types of plastics (PE, PP, PVC, PS, PET, PA, PU, PC, PMMA and POM) as target polymers for µRaman analysis.

Acknowledgments

This work is funded by the Austrian Federal Ministry of Labour, Social Affairs, Health, Care and Consumer Protection within the project “Microplastics in Breast Milk”, which we gratefully acknowledge.

Keywords: Microplastics, human breast milk, Raman microscopy

[Abstract:0475] [SERS/TERS/Plasmonics]

SERS-Based Assessment of Salinity in Hypersaline Solutions Supported by Dynamic Light Scattering

***Anamaria Couti*, Ecaterina Vlaico, Simona Pînzaru**

Ioan Ursu Institute of the Faculty of Physics, Babeș-Bolyai University, 1 Kogălniceanu 400084, Cluj-Napoca, Romania, RDI Institute in Applied Natural Sciences, Babeș-Bolyai University, 30 Fântânele 400327, Cluj-Napoca, Romania

Surface-Enhanced Raman Spectroscopy (SERS) is an ultrasensitive technique which is widely recognized for its applicability for the detection and quantification of molecules in extremely low concentrations. In this work, we expand its applicability to investigate the possibility of using SERS for the quantitative estimation of salinity in aqueous sodium chloride solutions which surpass the usual halide ions concentrations generally involved in silver nanoparticles (AgNPs) aggregation for SERS. Such hypersaline solutions apply to salt lakes and seawater.

We first used NaCl solutions with larger concentrations than usually employed for AgNPs aggregation in many SERS experiments to understand their aggregation behavior and to further correlate saline concentrations with the specific SERS band associated with Ag-Cl mode, as shown in Fig. 1. Saline solutions between 1 M and 2 M were prepared and mixed with classical, colloidal AgNPs as the SERS substrate. The intensity of this band was analyzed as a function of NaCl concentration over time, considering typical SERS temporal behavior. To estimate the salinity, the intensity of the specific peak was normalized to the O-H stretching band of water. The obtained intensity ratios were plotted against the NaCl concentration, and exponential fitting models were applied, with a maximum R^2 of 0.99. The evolution of the SERS signal over time was also studied to determine the optimal measurement time for reliable environmental applications.

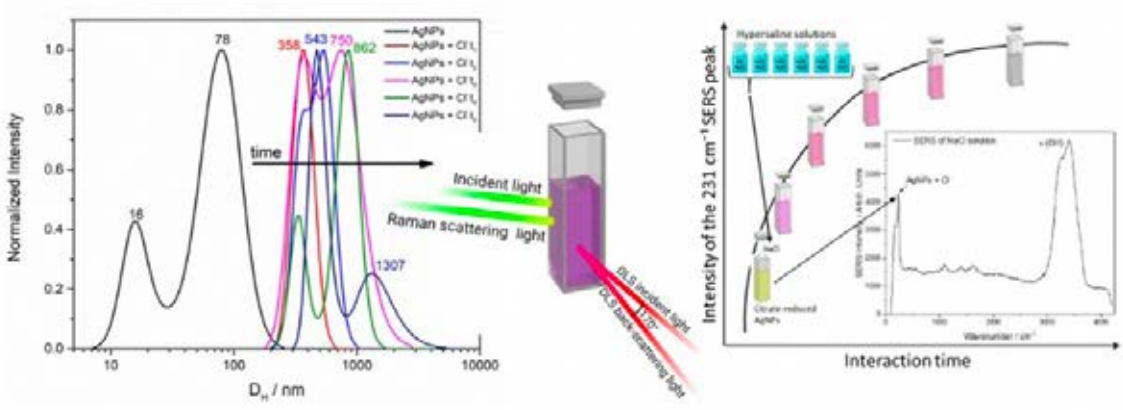
Dynamic light scattering (DLS) measurements were performed to examine the size distribution of the nanoparticles in the presence of hypersaline solutions. The DLS results show an increase in the hydrodynamic diameter with increasing time, indicating aggregation of the nanoparticles.

Secondly, we combined more reliable, environmentally relevant hypersaline solutions comprising both sodium chloride and sulfates, to resemble the salinity of real-world environmental samples.

These results suggest that SERS can be used as a promising approach for estimating salinity in hypersaline solutions.

Keywords: SERS, hypersaline waters, seawater, dynamic light scattering, silver nanoparticles

Fig.1. Combined SERS and DLS Analysis of Hypersaline Solutions Using AgNPs Aggregation



Posters

[Abstract:0477] [SERS/TERS/Plasmonics]

SERS as a Rapid Quality-Control Tool for Endotoxin Detection in Elastin-like Recombinamers

Lidia Asenjo Estevez[1], María Mayoral Yagüe[1], Raúl Escribano[3], Jose Antonio Manrique[1], Sergio Jiménez Blázquez[1], Sofía Julve[4], Ivan Reyes Rodriguez[1], Jaime García Concejo[2], Mercedes Santos Garcia[3], Javier Reguera[3], Marco Veneranda[1], Guillermo Lopez-Reyes[1]

[1]ERICA Research Group, University of Valladolid, Valladolid.
[2]Laboratory for Disruptive Interdisciplinary Science (LaDIS), University of Valladolid, Valladolid, Spain
[3]BIOFORGE Research Group, University of Valladolid, Valladolid
[4]AstraSpec S.L., Parque Tecnológico de Boecillo, Boecillo

Elastin-like Recombinamers (ELRs) are genetically engineered protein-based biomaterials with remarkable versatility for biomedical use. Their precise sequence control, intrinsic biocompatibility, stimuli responsiveness, and tunable self-assembly have made them attractive for applications such as controlled drug delivery, wound-healing scaffolds, vascular grafts, and regenerative medicine platforms. However, because ELRs are commonly produced through recombinant bacterial expression, they are exposed to the risk of residual endotoxin contamination, mainly lipopolysaccharides (LPS), which may strongly bias biological evaluation and trigger undesired inflammatory or immune responses even at low levels. Reliable, rapid, and structurally informative analytical approaches are therefore needed to complement routine endotoxin screening in ELR quality control.

In this work, surface-enhanced Raman spectroscopy (SERS) is explored as a rapid analytical strategy for identifying endotoxin-related spectral variations in ELR samples. SERS has already demonstrated strong sensitivity for LPS and other endotoxin-related signatures, making it a promising candidate for the analysis of subtle contamination phenomena in complex biomolecular systems. Pure and intentionally contaminated ELR samples were analysed by FTIR, conventional Raman spectroscopy, and SERS in order to compare their analytical performance. FTIR and spontaneous Raman spectroscopy confirmed the expected overall molecular structure of the ELR matrix, but their capacity to clearly discriminate endotoxin presence was limited, particularly when the polymer spectral contribution dominated the measurement.

By contrast, SERS provided the clearest analytical discrimination between pure and contaminated ELR samples. The spectra showed consistent and reproducible changes in relative band intensities, band positions, and local spectral profiles that were not resolved by FTIR or conventional Raman spectroscopy. These differences allowed a systematic distinction between uncontaminated and endotoxin-containing samples, indicating that SERS is sensitive to subtle molecular and interfacial alterations associated with contamination even when the ELR matrix dominates the overall vibrational response. The results therefore go beyond a preliminary indication of feasibility and demonstrate that SERS can deliver structurally meaningful contrast for endotoxin-related screening in recombinant biomaterials. This positions SERS as a particularly promising complementary tool for fast quality-control workflows in ELR production, with ongoing work now focused on customised nanoparticle synthesis, substrate optimisation, and multivariate modelling in order to further improve robustness, reproducibility, and classification performance.

Keywords: Surface-enhanced Raman spectroscopy (SERS), Elastin, Endotoxin, Raman

[Abstract:0482] [SERS/TERS/Plasmonics]

Copper Nanoparticles on Porous Silicon: A New UV-SERS Substrate

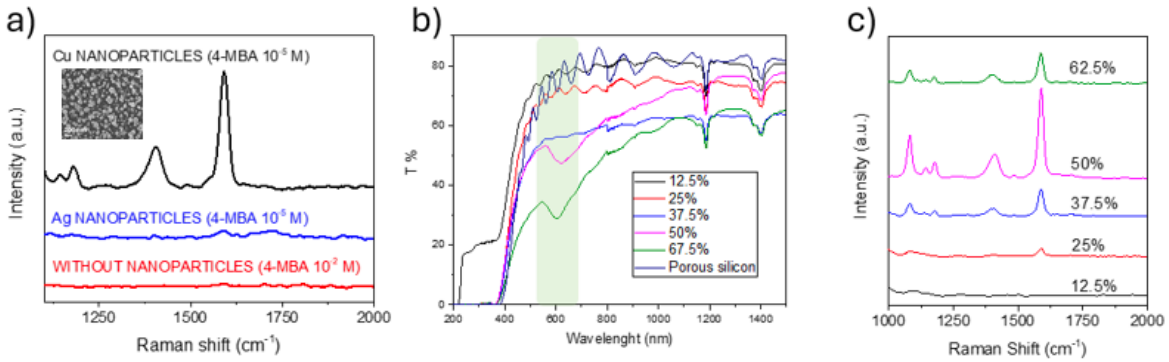
***Ettore Grimaldi*, Alessandro Chiadò, Paola Rivolo, Fabrizio Giorgis, Chiara Novara**

Department of Applied Science and Technology, Politecnico di Torino, Torino, Italy

Surface-enhanced Raman scattering (SERS) is a commonly used sensing technique in which inelastic light scattering by molecules is greatly enhanced due to their adsorption or chemisorption onto corrugated plasmonic surfaces, such as noble metal nanoparticles. This technique has several applications in the ultra-sensitive detection of biological molecules. The laser excitation wavelength typically falls in the visible or near-infrared (NIR) regions. Many biological and chemical molecules exhibit however absorption bands in the UV. For this reason, utilizing an UV excitation opens the possibility of increasing the sensitivity of the technique through resonance effects. This work investigates a strategy for the chemical growth of copper nanoparticles (NPs) on porous silicon, and their application as SERS substrates at 325 nm using a He-Cd laser. Although copper is known to exhibit a localized surface plasmon resonance around 590 nm, the experimental data here reported show that Cu nanoparticles provide SERS enhancement at 325 nm excitation. Taking into account that at the same excitation wavelength Ag nanoparticles don't exhibit a comparable enhancement, such effect could be attributed to a chemical enhancement mechanism. The metal nanoparticles are grown by immersion plating of a porous silicon (pSi)–polydimethylsiloxane (PDMS) membrane into a metal salt solution. The formation of copper on porous silicon was confirmed by UV-Vis-NIR spectroscopy and the nanomaterials were characterized by electron microscopy. An optimization of their chemical synthesis was carried out using 4-mercaptobenzoic acid (4-MBA) as probe molecule by evaluating the effect of several reaction parameters such as the solvent composition, type and concentration of metal precursor with the aim of obtaining the best possible SERS enhancement. Furthermore, a Design of Experiments (DoE) was performed to better optimize the CuSO4 concentration and the ethanol percentage in the solution, calculating the correlations between the two variables. Finally, the oxidation of the metal NPs was investigated with UV-Vis spectroscopy and SERS to exclude a possible role of copper oxide in the SERS enhancement. Overall, even if further characterizations are needed, the here proposed copper nanostructures showed promising results for SERS biosensing in the UV region.

Keywords: UV-SERS, Copper Nanoparticles, Porous Silicon

Spectroscopic characterization of Cu nanoparticles on porous silicon: SERS and optical response



a) Raman spectra of 4-MBA: comparison between measurements at 10^{-5} M in the presence of Cu (black) and Ag (blue) nanoparticles, and at 10^{-2} M in the absence of nanoparticles (red). The inset shows a representative FESEM image of the grown CuNPs; b) UV-Vis-NIR spectra of CuNPs synthesized at different percentages of ethanol in the aqueous solution. c) SERS spectra of 50 μM 4-MBA recorded on the same samples of b). All the SERS spectra were acquired at 325 nm laser beam excitation.

[Abstract:0483] [SERS/TERS/Plasmonics]

A Highly Sensitive SERS Strategy For Therapeutic Drug Monitoring Via InSitu Methylation And IodideDirected Enhancement

Yichun Chen, Yuting Fan, Jianfeng Wu, Kuo Qi, Jianwei Xie

Laboratory of Toxicant Analysis, Academy of Military Medical Sciences, Beijing, China

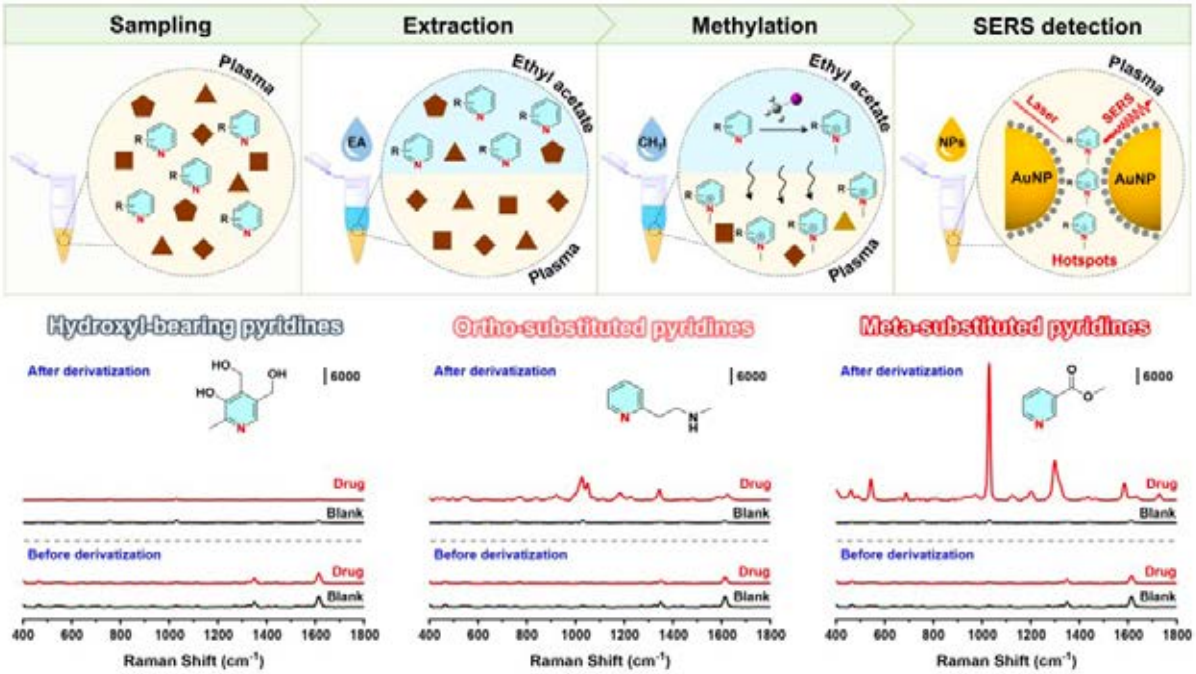
BACKGROUND: Therapeutic drug monitoring (TDM) plays a critical role in personalized medicine and in minimizing the risk of drug toxicity. Conventional detection techniques, represented by LC–MS/MS, are hindered by high costs, reliance on sophisticated equipment, and time-consuming operations. Consequently, there is an urgent need to develop convenient, stable, and high-resolution sensing technologies for TDM. Surfaceenhanced Raman spectroscopy (SERS) has emerged as a promising candidate for point-of-care testing (POCT), owing to its high sensitivity, rapid detection capability, and cost-effectiveness.

Experiments: In this work, motivated by the high prevalence of nitrogen heterocycles in FDA-approved small-molecule drugs (~82%, of which pyridines constitute 20%), we developed a universal SERS-based detection strategy. Methylation reagents were initially screened to enable efficient conversion of pyridine-containing drugs into corresponding pyridinium salts. To mitigate matrix interference in complex biological samples, an integrated sample pretreatment and detection method was further established. This method employs a "phase-transfer-like" process using ethyl acetate as the extraction solvent and iodomethane as the methylation reagent (Figure 1).

Results and DISCUSSION: LC–HRMS analysis confirmed efficient methylation of *meta*substituted pyridines (*e.g.*, methyl nicotinate), with conversion rates exceeding 90% at the pyridine nitrogen atom. In contrast, *ortho*-substituted or hydroxyl-bearing pyridine derivatives reacted preferentially at aliphatic amine or hydroxyl moieties, which restricted pyridinium formation and thus delineated the scope of the method. Using spiked plasma as a proof-of-concept sample, SERS fingerprint signals of *meta*-substituted pyridine drugs, obscured by the matrix background prior to derivatization, became clearly identifiable as distinct pyridinium peaks after methylation. Moreover, the detection sensitivity was enhanced by 10^4-fold compared to the underivatized analogs. For *ortho*-substituted analogs, sensitivity improved by 10^2fold, whereas hydroxylsubstituted derivatives exhibited negligible signal enhancement. These results verify that the pyridinium group is the key structural moiety responsible for signal amplification *via* electrostatic anchoring to the nanoparticle surface. Additionally, the entire detection workflow requires no complex pretreatment and can be accomplished within 10 minutes, making it suitable for rapid on-site testing. This work provides a novel, field-deployable strategy with considerable potential for the development of universal and rapid drug-monitoring platforms.

Keywords: SERS, Therapeutic drug monitoring, Methylation, Pyridines, On-site detection

Figure 1. Schematic illustration of the SERS strategy for therapeutic drug monitoring via insitu methylation and iodidedirected enhancement



Posters

[Abstract:0484] [SERS/TERS/Plasmonics]

Three-dimensional Hierarchical Nanowire-Networks with Deep-Focus Tolerance and Adhesion Robustness For Harsh-Environment SERS Sensing

Jinglai Duan

State Key Laboratory of Heavy Ion Science and Technology, Institute of Modern Physics, Chinese Academy of Sciences

With growing demand for field-deployable and reliable Surface-Enhanced Raman Scattering (SERS) applications, a critical yet often overlooked challenge is the stringent requirement for precise laser focusing, which severely limits operation outside controlled laboratory environments. To overcome this focal precision barrier, we present a three-dimensional (3D) hierarchical Au nanowire network (NWNW) engineered as a robust SERS substrate. Its architecture is engineered to provide exceptional deep focus tolerance, exhibiting pronounced 3D optical activity along the z-direction and angular anisotropy under polarized illumination. This enables the substrate to achieve an ultralow detection limit of 1×10-12 M for non-resonant 4-mercaptopyridine molecules, while maintaining outstanding signal uniformity and repeatability (relative standard deviation, RSD <10%). Moreover, an effective medium model reveals that the synergistic interplay between increased light scattering rates, elevated local density of optical states, and broadened eigenmodes jointly contributes to efficient light harvesting and near-field enhancement throughout the 3D architecture. Equally importantly, the nanowire-network is mechanically reinforced by an integrated nanogrid framework, thereby ensuring adhesion stability and stable SERS performance even when subjected to harsh environments. By solving the focal precision challenge while maintaining robustness, this work demonstrates that the 3D Au NWNW is not only a highly sensitive SERS substrate but also a viable platform for transitioning SERS from controlled laboratory environments towards demanding real-world applications.

Keywords: 3D nanowire networks, surface-enhanced Raman spectroscopy, deep-focus tolerance, adhesion robustness, effective medium model

[Abstract:0486] [Biology/Biomedicine]

AI-Driven Raman Spectroscopy for Robust Pathogen Identification, Microbial Load Validation, and Clinical Antibiotic Resistance

***Amr A. Nassrallah*[1], *Helal A. Suleiman*[2], *Rami Zewail*[3], *Marwan A. Farag*[4], *Ahmed Abdel Mawgood*[1], *Sameh A. Awad*[5], *Badawi Anis*[6], *Samir F. El Mashtoly*[7]**

[1]*Biotechnology department, Faculty of Basic and Applied Science, E-JUST, New Borg El-Arab, Egypt*
[2]*Faculty of Computers and Artificial Intelligence, Capital University, Egypt*
[3]*Department of Computer Science & Engineering, Egypt-Japan University of Science and Technology (E-JUST), New Borg El Arab, Alexandria, Egypt*
[4]*Faculty of Computer Science & Information Technology, Helwan National University, Cairo, Egypt*
[5]*Department of Dairy Science and Technology, Faculty of Agriculture, Alexandria University, Egypt*
[6]*Spectroscopy Department, Physics Research Institute, National Research Centre (NRC), Giza, Egypt*
[7]*Leibniz Institute of Photonic Technology, Albert-Einstein-Strase 9, Jena, Germany*

There is a growing interest in leveraging artificial intelligence for the rapid, label-free identification of bacterial pathogens via Raman spectroscopy. However, traditional models often struggle with high-dimensional noise and the misclassification of closely related species. In this work, we present a robust identification framework utilizing a Residual Neural Network (ResNet) backbone optimized with a hybrid Contrastive Loss and Label Smoothing objective to prevent model overconfidence and enhance generalization. We further validate this Raman-based platform against gold-standard quantitative real-time PCR (RT-PCR) and evaluate its performance in clinical antibiotic resistance scenarios.

RESULTS: The hybrid training objective significantly enhanced classification performance, specifically resolving critical bottlenecks such as the misclassification of Salmonella enterica. By softening training targets via Label Smoothing, the model achieved a 99.64% accuracy 1 on reference data and successfully identified 51 true samples that baseline cross-entropy models failed to recognize. To ensure real-world reliability, Raman spectral intensities were benchmarked against quantitative RT-PCR, showing high correlation across varying microbial loads for E. coli, S. aureus, and S. enterica (Figure 1). Finally, the system's performance in clinical antibiotic resistance scenarios confirmed minimal performance drift and high accuracy for Vancomycin, Penicillin, and Ciprofloxacin, demonstrating robust knowledge retention even after sequential updates (Figure 2).

Keywords: Raman Spectroscopy, Food Safety, RT-PCR Validation, Antibiotic Resistance, Label Smoothing.

Figure 1

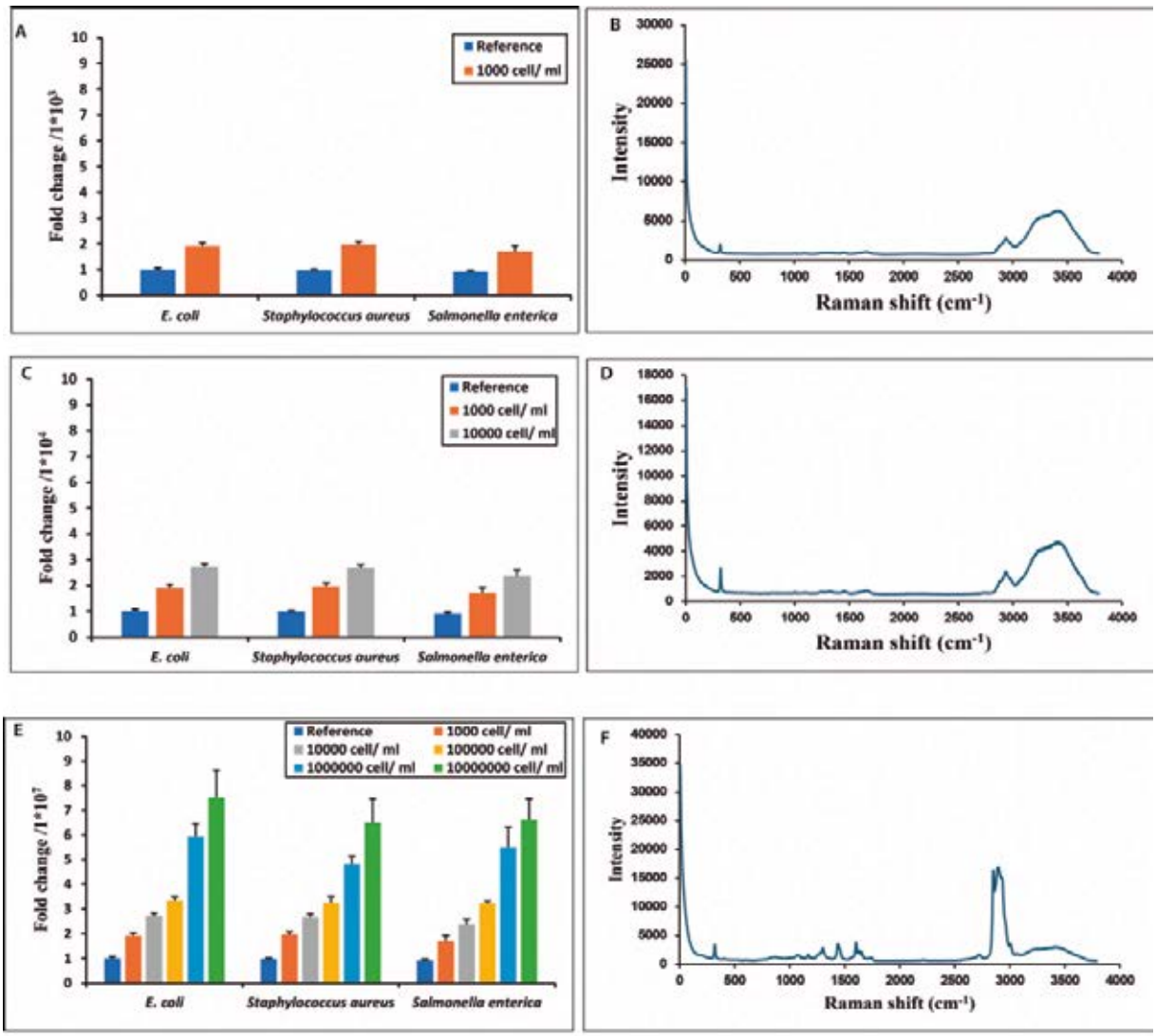
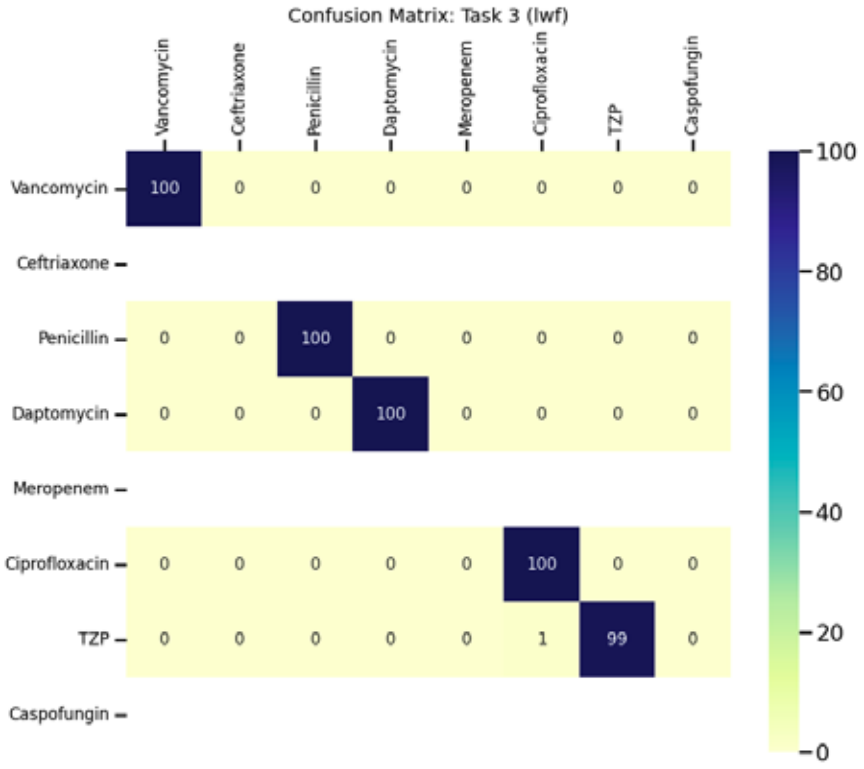

A
Reference
1000 cell/ ml
Fold change /1*10³
E. coli
Staphylococcus aureus
Salmonella enterica
B
Intensity
Raman shift (cm⁻¹)
C
Reference
1000 cell/ ml
10000 cell/ ml
Fold change /1*10⁴
E. coli
Staphylococcus aureus
Salmonella enterica
D
Intensity
Raman shift (cm⁻¹)
E
Reference
1000 cell/ ml
10000 cell/ ml
100000 cell/ ml
1000000 cell/ ml
10000000 cell/ ml
Fold change /1*10⁷
E. coli
Staphylococcus aureus
Salmonella enterica
F
Intensity
Raman shift (cm⁻¹)

Figure 2


Confusion Matrix: Task 3 (lwf)
Vancomycin
Ceftriaxone
Penicillin
Daptomycin
Meropenem
Ciprofloxacin
TZP
Caspofungin
100
80
60
40
20
0

[Abstract:0491] [Planetary/Geosciences]

Lizardite's Crystallographic Orientation Elucidated by Raman Spectroscopy

***Jeremy S. Rooney*[1], *Matthew S. Tarling*[3], *Keith C. Gordon*[1], *Steven A. F. Smith*[2], *Marianne Negrini*[2]**

[1]*Department of Chemistry, University of Otago, Dunedin, New Zealand*
[2]*Department of Geology, University of Otago, Dunedin, New Zealand*
[3]*Department of Earth, Ocean and Atmospheric Sciences, University of British Columbia, Vancouver, Canada*

Serpentinites are a common rock type that are primarily composed of serpentine minerals ($Mg_3Si_2O_5(OH)_4$). There exist four common forms of serpentine: lizardite, chrysotile, antigorite and polygonal serpentine. Each form has a distinct structure that is a means of accommodating a slight lateral mismatch between the tetrahedral silicate sheet and octahedral magnesium sheet that make up a T-O layer.

Over the course of several Raman measurements of serpentinite thin sections, it was observed that there were significant shifts in the main O-H stretching frequency of lizardite - this was also observed occasionally throughout the literature.[1] While initially attributed to metal cation substitution distorting the lattice, it became apparent from scanning electron microscopy with energy dispersive spectroscopy (SEM-EDS) that there was insufficient compositional differences between crystals within most samples to account for such shifts (ca. 14.5 cm^{-1}).

A summary of results from our recent publication are presented whereby it was determined that the O-H peak shifts were dependent on the inclination of lizardite's c-axis relative to the impinging laser.[2] This was determined through Raman measurements on polycrystalline thin sections whose grains had their orientations independently determined by electron backscatter diffraction (EBSD). Additionally, Raman measurements were taken on a single crystal mounted on a spindle stage that permitted the inclination of the c-axis to be accurately altered.

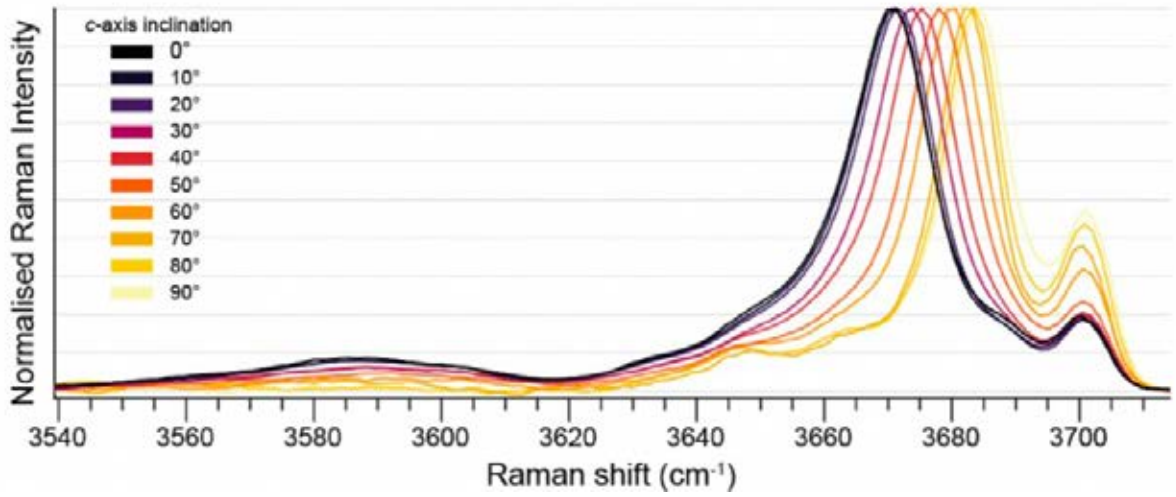
References:

[1] Compagnoni, R.; Cossio, R.; Mellini, M. Raman Anisotropy in Serpentine Minerals with a Caveat on Identification *J. Raman. Spectrosc.* 2021, 52*(7)*, 1334-1345.

[2] Tarling, M. S.; Demurtas, M.; Smith, S. A. F.; Rooney, J. S.; Negrini, M.; Viti, C.; Petriglieri, J. R.; Gordon, K. C. Crystallographic orientation mapping of lizardite serpentinite by Raman spectroscopy *Eur. J. Mineral.* 2022, 34*(3)*, 285-300.

Keywords: Serpentine, Crystalline, Orientation

Figure 1



Hydroxyl blue shift based on incline.

[Abstract:0494] [Materials]

Substrate-Dependent Correlation Between Raman Signatures and Terahertz Conductivity in Single-Layer Graphene

***Fatma Feyza Sadıkoğlu*, Yusuf Samet Aytekin, Okan Esentürk**

Department of Chemistry, Middle East Technical University (METU), Ankara, Türkiye

Substrate-induced effects critically influence both the spectroscopic and electronic properties of single-layer graphene. In this study, single-layer graphene transferred onto different dielectric substrates was systematically investigated using Raman spectroscopy and optical pump terahertz probe spectroscopy (OPTP).

Raman measurements were performed using a 532 nm excitation under identical instrumental conditions, and spectra were collected from five different locations on each sample to assess spatial homogeneity. The analysis focused on the characteristic graphene bands and the intensity ratio I(2D)/I(G) to evaluate layer quality and uniformity. Among the investigated substrates, graphene on PDMS+PMMA exhibited the highest I(2D)/I(G) ratio of 2.

Terahertz (THz) radiation lies between the microwave and infrared regions (0.1–10 THz) and is sensitive to low-energy processes such as charge carrier dynamics and phonons. Terahertz time-domain spectroscopy (THz-TDS) enables direct measurement of ultrafast THz pulses, allowing extraction of amplitude and phase information. Optical pump–terahertz probe (OPTP) spectroscopy extends this approach by introducing an optical excitation pulse followed by a delayed THz probe, enabling tracking of carrier dynamics on picosecond timescales.

In this study, OPTP was used to monitor charge carrier behavior of the graphene samples. Figure 1a presents fluence normalized 800 nm pump THz probe spectra of samples: single-layer graphene (1LG) on PET, PDMS, and PDMS+PMMA substrates. All samples exhibited a positive THz response, indicating decreased conductivity upon photoexcitation, which is typical for single-layer graphene. The PDMS+PMMA sample showed the highest THz conductivity among the three.

These results are consistent with Raman spectra (Figure 1b), where the PDMS+PMMA sample exhibited an I(2D)/I(G) ratio of 2, characteristic of single-layer graphene. The other samples, with lower THz conductivity, showed ratios of 1.34 and 0.13, indicating multilayer structures. This non-uniform multilayer nature may act as defects and reduce charge carrier mobility.

Keywords: Single-layer graphene, Raman spectroscopy, Terahertz spectroscopy (OPTP), Substrate effects, Carrier dynamics

[Abstract:0496] [Theory/Computation]

Piezoelectricity of the β phase of PVDF: Investigating the Molecular Mechanism and the Role of Intermolecular Interactions Using Density Functional Theory and Raman Spectroscopy

***Gianluca Serra*, Alessia Arrigoni, Mirella Del Zoppo, Chiara Castiglioni, Matteo Tommasini**

Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta", Politecnico di Milano, Milan, Italy

Poly(vinylidene fluoride) (PVDF) is one of the most studied piezoelectric polymers: when its β phase, one of its many crystalline polymorphs, is mechanically deformed, it produces an electric potential difference. This makes PVDF a functional material with several applications in technology. However, the precise molecular mechanism governing the piezoelectricity of the β phase of PVDF is still elusive. In particular, the role of intermolecular interactions has received little consideration.

Here, we present an investigation of the molecular mechanism of the piezoelectricity of the β phase of PVDF based on quantum chemical computations and Raman spectroscopy. We first compute the equilibrium Raman spectrum of the system within periodic-boundary-conditions density functional theory, and assign the experimental spectrum of samples with large content of β phase. In particular, we model our system both as a one-dimensional infinite chain and a three-dimensional periodic crystal. Then, we study the effect of intermolecular interactions on the equilibrium Raman spectrum. To do so, we construct two series of dilated models obtained by imposing fixed dilations of either one or two non-axial cell parameters. This allows us to selectively remove intermolecular interactions and observe their effect on vibrational frequencies and Raman intensities. The variation of the equilibrium Raman spectrum with changing intermolecular interactions serves as a proxy of the modification of the potential energy surface upon mechanical deformation.

We obtain computational insight on the role of intermolecular interactions both on the energy landscape of a single polymer chain and on the systems' vibrational properties. Assigning the experimental Raman spectrum of PVDF, we find that the periodic one-dimensional model misses some important features of the real system: thus, a three-dimensional model is mandatory for studying the vibrational properties of the β phase of PVDF. Second, we show how the frequencies and intensities of crystal Raman-active modes are selectively affected by intermolecular interactions, that in most cases show long-range effects.

All of this supports a view in which the piezoelectricity of the β phase of PVDF can be explained in terms of the rotation of a single polymeric chain within the crystal, with such rotation largely affected by intermolecular interactions.

Keywords: density functional theory, periodic boundary conditions, intermolecular interactions, crystal polymorphs, piezoelectricity

[Abstract:0503] [SERS/TERS/Plasmonics]

Non-aqueous SERS Detection Enabled by Hexadecylamine-capped Ag Bumpy Nanoshells

***Sungjun Kwak*[1], *Dae Hong Jeong*[2]**

[1]*Department of Chemistry Education, College of Education, Seoul National University, Seoul, Republic of Korea*
[2]*Department of Chemistry Education, College of Education, Seoul National University, Seoul, Republic of Korea, Learning Science Research Institute, Seoul National University, Seoul, Republic of Korea*

Surface-enhanced Raman spectroscopy (SERS) is typically limited to aqueous environments and thiol-based adsorption, restricting its applicability to a narrow range of analytes. Here, we demonstrate a non-aqueous SERS platform based on hexadecylamine (HDA)-capped silver nanoshells that enables the detection of structurally diverse non-thiol molecules. The loose organic interface provided by HDA facilitates molecular access and stabilizes adsorption in ethanol, overcoming the limitations of conventional citrate-capped nanoparticles. A systematic study using several representative molecules with varying hydrophobicity and functional groups reveals that non-aqueous environments allow both improved molecular dispersion and enhanced interfacial accessibility. Molecules containing hydroxyl and carbonyl functionalities exhibit stable adsorption and reproducible SERS signals, while non-functionalized aromatics show minimal interaction. Furthermore, the platform supports robust detection of more complex dye molecules, including alizarin and purpurin, demonstrating its applicability beyond simple model compounds. These results highlight the critical role of solvent and interfacial structure in governing SERS detectability. By decoupling molecular accessibility from aqueous constraints, this work establishes a general strategy for extending SERS measurements to non-aqueous systems and broadening the range of detectable chemical species.

Keywords: non-aqueous, SERS, nanoparticle, hexadecylamine, functional group

[Abstract:0505] [SERS/TERS/Plasmonics]

Synthesis and Performance Evaluation of Anisotropic Silver Coated Nanoworms for SERS Based Trace Detection of Crystal Violet And Ammonium Nitrate

***Zeynep Cantürk*, Ghazanfar Ali Khan, Alpan Bek**

Department of Physics, Middle East Technical University, 06800, Ankara, Türkiye

Silver (Ag) coated nanostructures (NSs) hold significant potential for trace molecule detection using surface-enhanced Raman scattering (SERS) spectroscopy due to their excellent plasmonic characteristics. Nevertheless, the impact of Ag coating on nanoworms (NWs), especially in the context of SERS applications, is still not well studied. In this research, we present a highly anisotropic Ag shell on NWs that demonstrates exceptional SERS sensitivity. The undulating shape of the NWs, along with the optimized reaction conditions during the seeded growth method, facilitated the creation of a highly anisotropic Ag shell on NWs without leading to secondary nucleation within the growth solution. Finite element simulations indicated that these Ag coated NWs (Ag@NWs) provide superior field enhancement compared to the NWs, and they also exceed the performance of smoother Ag ellipsoids when in aggregate form. A strong comparison of the SERS capabilities between NWs and Ag@NWs was established using crystal violet. The Ag@NWs exhibited an experimental enhancement factor that is 3.5 times greater than that of NWs, achieving detection limits of ten picomolar for crystal violet and ten micromolar for ammonium nitrate. These findings indicate that an anisotropic Ag shell can greatly enhance the SERS performance of NWs, making it an engineered ultrasensitive nanomaterial suitable for quantitatively detecting trace levels of analytes.

Keywords: nanoworms, gold-silver core-shell nanoworms, anisotropic silver shell, surface-enhanced Raman scattering, trace level SERS detection

[Abstract:0509] [SERS/TERS/Plasmonics]

Background-Free, Label-Free, and Reproducible SERS via Plasma–Halide-Engineered Gold Nanoparticles

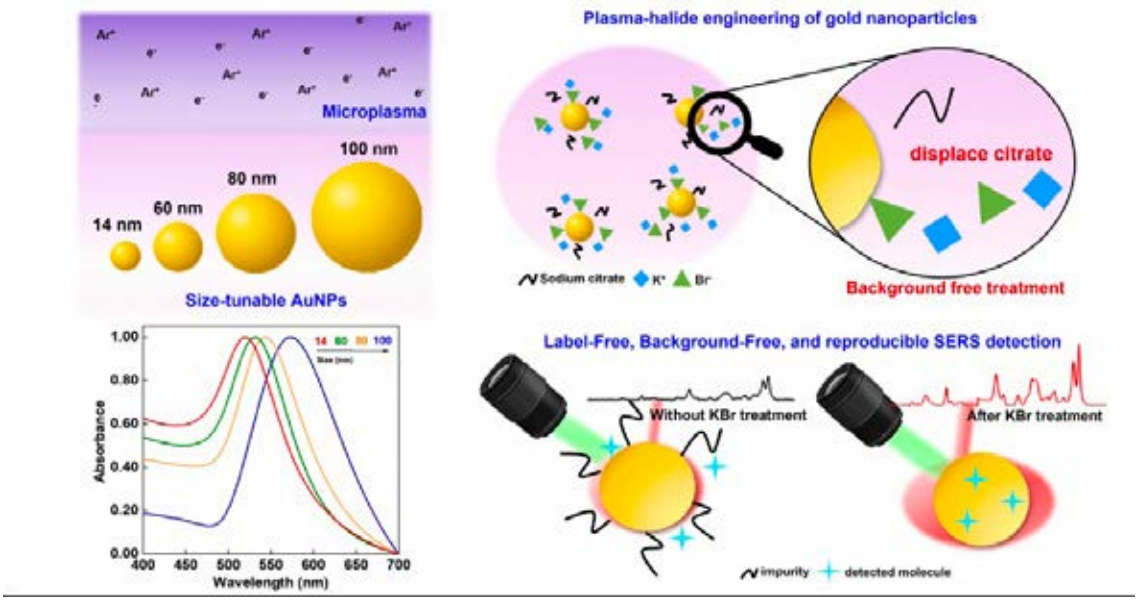
***Yen Ling Chiu*, Ya Chi Chen, Loid Elizabeth Urtecho Navas, Wei-Hung Chiang**

Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei City, Taiwan

Surface-enhanced Raman spectroscopy (SERS) is often limited by substrate-derived background from organic ligands (e.g., citrate), which degrades spectral fidelity, sensitivity, and quantitation. We report a measurement-oriented SERS platform based on size-tuned, microplasma-synthesized gold nanoparticles (AuNPs, 14–100 nm) that are surface-purified with bromide (Br^-). Bromide competitively displaces weakly bound citrate while remaining Raman-inactive, thereby suppressing baseline features in the 1000–1800 cm^{-1} fingerprint region without introducing new peaks. An optimal Br^- window (~1.5 mM, ~3 h) achieves effective cleaning while avoiding surface passivation. The resulting substrates deliver strong enhancement (EF > 10^6), sub-nanomolar limits of detection (10^{-9} M for rhodamine 6G; 10-10 M for malachite green), and wide linear ranges (10-9–10^{-4} M and 10^-10–10^{-4} M, respectively). Spot-to-spot variability is low (RSD < ~8%), and activity is retained over weeks (>90% signal after storage), underscoring practical reproducibility and stability. Spectroscopic and surface-charge analyses corroborate ligand displacement and improved adsorption on clean Au surfaces while preserving plasmonic response. This simple, green, and scalable plasma–halide strategy provides background-free, label-free, and reproducible SERS measurements. Driven by electrostatic complementarity, this platform offers a highly effective route for the quantitative trace analysis of cationic analytes, relevant to environmental monitoring and chemical safety.

Keywords: Surface-enhanced Raman scattering, nanoparticles, plasma synthesis, nanotechnology, sensor.

Two-step synthesis of clean-surface, size-tunable gold nanoparticles (AuNPs) for low-background SERS detection of environmental pollutants.



AuNPs of tunable sizes were rapidly synthesized via an ambient microplasma technique, followed by potassium bromide (KBr) treatment to eliminate surface-bound citrate and suppress background signals. The halide-treated AuNPs exhibited enhanced SERS performance due to improved electrostatic interactions with target analytes.

Posters

[Abstract:0518] [SERS/TERS/Plasmonics]

Three-Dimensional Nanostructured Silicon substrate like a Nano-grass Arrays for Surface Enhanced Raman Spectroscopy Applications

***Munizer Purica*, Octavian Simionescu, Andrei Avram,**
Florin Constantin Simionescu, Stefan Caramizoiu, Gabriel Craciun

National Institute for R&D for Microtechnologies – IMT Bucharest; Department for Scientific and Technological Research, Bucharest, Romania

Surface Enhanced Raman Spectroscopy (SERS) has contributed decisively to extending the applications of standard Raman spectroscopy to the molecular level. The abilities to control the shape, orientation, arrangement of silicon nanostructures on the surface using nanofabrication techniques have led to the realization of dimensionally well-defined nanostructures and ultimately to the increase of the efficiency factor (EF-Enhanced Factor) of molecular level detection. We present a plasmonic-active 3D-SERS substrate based on silicon nano-grass arrays achieved by dry etching, in sulfur hexafluoride and oxygen (SF6:O2) plasma, of n-Si (100) wafers (diameter 100 mm) with the Plasmalab System 100. The system is of the Inductively Coupled Plasma Deep Reactive Ion Etching (ICP DRIE). The dimensional design of the vertical silicon nanostructures was based on simulation/modeling with the OptiFDTD software on the analysis of the LSPR effect considering the geometric dimensions of the one dimensional nanostructure (nanowires) and the thickness of the deposited metal. The simulations were performed considering a cylindrical layout for the vertical nanostructures arrays with a metal coverage of 33% of the height and for excitation wavelengths -633 nm, 532 nm and 488 nm. The best results for the enhancement of the plasmonic effect (electric field) were obtained for vertical nanostructures arrays with the characteristics: height of 4.5 mm, diameter of 60 nm, metal (Au or Cu) coverage at a distance of 150 nm from the tip and the distance between them of 30 nm. The technology for obtaining Si 1D vertical nanostructure by DRIE and maskless was optimized to allow the achievement of dimensions below 5 mm the height of the wires and less than 100 nm diameter and distances between them, favorable dimensions for SERS applications.

The metal films (Au, Ag) of 15 nm thickness were deposited on nanostructures by electron beam induced evaporation at low pressures. The SERS substrate functionality was performed using LabRAM HR 800 spectrometer. The sample consists of ammonium nitrate /NH4NO3 dissolved in water, a dilution of 20 mg/L (1.2x10-4M) by monitoring the Raman line characteristic of the NO3 group positioned at ~1060 cm-1 (detected only using the fabricated SERS substrate).

Keywords: SERS, silicon,Nano-grass, arrays

[Abstract:0519] [Biology/Biomedicine]

Raman Spectroscopy Approaches for Early Detection of Gynaecological Cancer Using Liquid Biopsy

***Thaara Rose Wilson*[1], *Irene Narinda*[3], *Lauren Mcmahon*[3], *Aidan Meade*[2], *Sharon O'toole*[3], *Fiona Lyng*[1]**

[1]*Radiation and Environmental Science Centre (RESC), Physical to Life Sciences Research Hub, Technological University Dublin, Ireland*
[2]*School of Physics & Clinical & Optometric Sciences, Technological University Dublin, Ireland*
[3]*Trinity Translational Medicine Institute, Trinity Centre for Health Sciences Trinity College Dublin, St James's Hospital, Dublin, Ireland*

INTRODUCTION: A critical diagnostic gap exists in gynaecological oncology, where the absence of non-invasive screening tools precludes reliable early-stage detection. Ovarian cancer lacks an effective population-based screening test, with over 70% of cases detected at FIGO stage III–IV. For endometrial cancer, current diagnostic pathways rely on imaging and invasive tissue sampling. A minimally invasive liquid biopsy capable of detecting molecular alterations early would offer substantial clinical benefit. This study primarily evaluates the diagnostic capacity of Raman spectroscopy (RS) to discriminate between gynaecological malignancies and benign gynaecological conditions. Both serum and plasma were compared using multivariate models. Additionally, this study evaluates the impact of pre-analytical handling on spectral integrity to ensure clinical translatability.

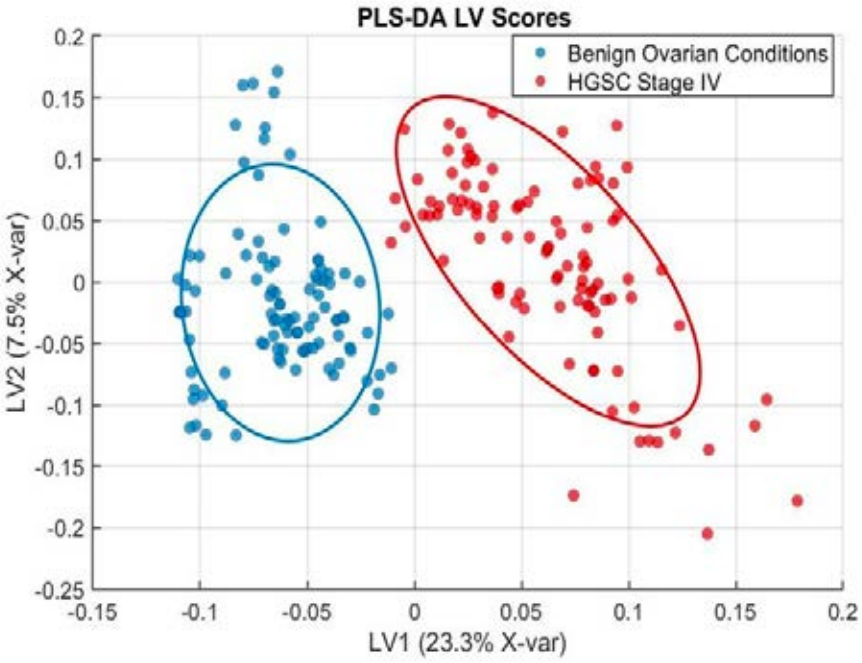
Materials & METHODS: Matched plasma and serum samples were collected from patients (n=80) with High-Grade Serous Ovarian Carcinoma (HGSC), Endometrioid Endometrial Adenocarcinoma and benign gynaecological conditions. All samples were analysed in their native liquid state. Raman measurements (785 nm source, 60× water immersion objective) were performed on 50 µL samples using a Horiba-Jobin-Yvon LabRAM HR800 spectrometer. Ten spectra per sample were recorded and pre-processed prior to data analysis. Principal Component Analysis (PCA) and Partial Least Squares Discriminant Analysis (PLS-DA) were employed for multivariate classification. The influence of freeze-thaw cycles, anticoagulants, and haemolysis were also investigated.

RESULTS: Raman spectra remained stable across anticoagulants and controlled freeze-thaw cycles; however, rapid sample thawing and haemolysis induced spectral shifts indicative of protein conformational changes. For HGSC (Stage IV), 100% specificity was achieved in both biofluids, with serum yielding a superior 93.5% F1-score. Discriminating features included elevated nucleic acid signals, consistent with increased cell turnover and ctDNA, and reduced carotenoid levels indicative of oxidative stress. For early-stage (Stage IA) Endometrial Adenocarcinoma, serum samples achieved a 95.5% F1-score. These samples exhibited enhanced glycogen and lipid/glycoprotein signatures, characteristic of early metabolic adaptation in malignancy. Across all metrics, serum consistently outperformed plasma.

CONCLUSION: The high classification accuracy for both malignancies underscores the potential of Raman spectroscopy as a rapid, non-invasive diagnostic tool for gynaecological oncology. Furthermore, this study demonstrates that rigorous control of pre-analytical variables is essential for the reproducible clinical implementation of Raman-based liquid biopsies.

Keywords: Raman spectroscopy, Liquid biopsy, Gynaecological oncology, Endometrial cancer, Ovarian cancer, Pre-analytical variables

Serum PLS-DA LV Score Plot



The PLS-DA score plot demonstrates a clear separation between HGSC Stage IV (red) and Benign Ovarian Conditions (blue) along the first Latent Variable (LV1).

[Abstract:0522] [Novel Approaches]

Coupling Raman Spectroscopy with Electrochemistry for Monitoring DTNB Reduction on a 3D-Printed Electrode

***Elif Çalık Kayiş*[1], *Tugba Tezcan*[1], *Ahmet Furkan Kayiş*[2], *Özcan Yalçınkaya*[2], *Ugur Tamer*[1]**

[1]*Faculty of Pharmacy, Department of Analytical Chemistry, Gazi University, 06330 Ankara, Turkey*
[2]*Faculty of Science, Department of Chemistry, Gazi University, 06500 Ankara, Turkey*

Ellman's reagent (5,5′-dithiobis-(2-nitrobenzoic acid)) (DTNB) is a widely used redox-active compound due to its reduction to 2-nitro-5-thiobenzoate (TNB) (Scampicchio et al., 2007). DTNB has also been widely used as a label in numerous studies for both Raman and electrochemical applications (Gumustas et al., 2018; Kayiş et al., 2025; Panhwar et al., 2020). In this study, a multimodal approach combining electrochemistry and Raman spectroscopy is presented to monitor and confirm the reduction of DTNB on a 3D-printed electrode surface. The integration of these two techniques enables both real-time electrochemical characterization and molecular-level spectroscopic validation. A conductive 3D-printed electrode was fabricated and used as the working electrode in a three-electrode system. The electrochemical reduction behavior of DTNB was investigated using cyclic voltammetry and differential pulse voltammetry in an appropriate buffer medium. The reduction process was characterized by a distinct cathodic peak corresponding to the cleavage of the disulfide bond and was associated with the formation of TNB. The obtained electrochemical data were evaluated in terms of peak potential, current intensity, and scan rate dependence, providing insight into the reaction mechanism. Raman spectroscopy was employed as a complementary technique to confirm the formation of TNB. Comparison of Raman spectra recorded before and after electrochemical reduction revealed characteristic spectral changes corresponding to the conversion of DTNB to TNB. In particular, variations in bands associated with thiolate groups and aromatic ring vibrations clearly indicated the reduction process. The agreement between electrochemical signals and Raman spectral data demonstrates the effectiveness of this dual-technique approach. This study demonstrates that the combined use of Raman spectroscopy and electrochemical techniques provides a powerful strategy for monitoring redox reactions. The advantages of 3D-printed electrodes, such as low cost, design flexibility, and rapid fabrication, make them attractive platforms for sensing applications. The proposed methodology offers a robust foundation for the development of integrated electrochemical–spectroscopic sensors and can be extended to more complex biological and analytical systems

Keywords: Raman spectroscopy, electrochemical reduction, DTNB, 3D-printed electrodes, multimodal analysis

[Abstract:0523] [Biology/Biomedicine]

Multivariate Spectroscopic Characterization of Canine Cancer: Identification of Molecular Fingerprints

***Arti Hole*[1], *Kiran Bendale*[2], *Sagar Barge*[3], *Pradip Chaudhari*[2], *Murali Krishna Chilakapati*[1]**

[1]*Chilakapati Laboratory, ACTREC, TMC, Navi Mumbai, Maharashtra,410210 India*
[2]*Comparative Oncology Program, ACTREC, TMC, Navi Mumbai, Maharashtra, 410210 India*
[3]*Amity Institute of Biotechnology, Amity University, Maharashtra, Mumbai, 410206 India*

Cancer is a significant health risk to dogs, requiring accurate, timely diagnosis to improve outcomes [1]. Prognoses rely on veterinary consultation and symptom monitoring, as early detection enhances therapeutic intervention [2,3]. While tissue biopsy remains the gold standard, it is unsuitable for early detection or repeated monitoring [4]. Serum Raman spectroscopy (RS) offers a label-free, non-destructive alternative, providing a biochemical fingerprint of samples [5]. This technique uses inelastic light scattering to detect molecular vibrations, identifying structural changes associated with cancer. In this study, 27 canine serum samples were categorised into normal (n=9), skin cancer (n=9), and breast cancer (n=9) groups. Samples were analysed using a Raman confocal microscope (Raman alpha300R, WITEC GmbH, Germany) with a 633 nm laser at 28 mW. Excitation was focused through a 100× objective lens (Zeiss, 0.75 N.A.). Raman photons were collected via a 50 µm optical fibre, directed into a 300 mm spectrograph with a 600 grooves/mm grating and a thermo-cooled CCD detector. Spectral acquisition used a 15-second integration time; five accumulations were averaged to improve the signal-to-noise ratio. The 0.75 µm spectral resolution resolved detailed features. Raw spectra underwent baseline correction, smoothing, and normalisation before being averaged to generate representative profiles. Multivariate statistical analysis interpreted the data. Principal component analysis (PCA) reduced dimensionality, and Principal Component linear discriminant analysis (PC-LDA) developed a model differentiating normal, skin cancer, and breast cancer samples. The PC-LDA model demonstrated 78% accuracy, indicating potential for serum RS as a diagnostic tool for canine cancer. Significant intensity differences occurred at 1650, 1450, 1250, 1005, and 650 cm^{-1}. These variations likely correspond to molecular alterations in protein structures linked to cancer pathology, highlighting the biochemical basis for the observed performance.

Keywords: Raman Spectroscopy, Canine cancer, Multivariate analysis, PCA, PC-LDA.

[Abstract:0525] [SERS/TERS/Plasmonics]

Comparative Study on the Effect of Substrate Structure Type and Laser Wavelength on SERS Performance

Ayse Mine Saridag

Gaziantep University

Surface-enhanced Raman scattering (SERS) is a powerful analytical technique that significantly amplifies Raman signals of molecules adsorbed onto nanostructured noble metal surfaces. The efficiency of SERS depends on several key parameters, such as the size, shape, type, and aggregation state of nanoparticles, as well as the wavelength of the excitation laser. Optimization of these factors is crucial for maximizing SERS enhancement and achieving sensitive detection. In this study, we systematically investigate the relationship between SERS substrate structure and laser wavelength by preparing both two-dimensional (2D) and three-dimensional (3D) SERS substrates from colloidal silver and gold nanoparticles. Both 2D and 3D substrates were fabricated using concentrated colloidal dispersions, and their SERS activities were tested using two different laser wavelengths (514 nm and 830 nm). The substrates were characterized by UV-Vis spectroscopy and scanning electron microscopy (SEM). Rhodamine 610 was used as a probe molecule to evaluate SERS activity. Our results show that the structural configuration of colloidal nanoparticle-based substrates and the choice of laser wavelength critically affect SERS performance. This study provides valuable guidance for the design and optimization of effective SERS platforms for advanced analytical applications.

Keywords: SERS, Nanostructure, Laser Wavelength

[Abstract:0527] [SERS/TERS/Plasmonics]

Comprehensive SERS Characterization of Multi-Class Pharmaceutical Micropollutants

Sylwia Magdalena Berus*, *Aneta Aniela Kowalska*, *Agnieszka Kamińska

Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw 01-224 Poland

Pharmaceutical compounds released into aquatic environments represent a growing global concern due to their potential impact on ecosystems and human health. Among the most frequently detected contaminants are antibiotics (e.g. sulfamethoxazole or clarithromycin), non-steroidal anti-inflammatory drugs (NSAIDs) e.g. diclofenac, and antipsychotics e.g. amisulpride — structurally and pharmacologically diverse molecules that pose significant analytical challenges. Conventional detection methods, such as HPLC-MS, offer high sensitivity but require sophisticated instrumentation and complex sample preparation, highlighting the need for rapid and cost-effective alternatives.

In this work, Surface-Enhanced Raman Spectroscopy (SERS) was used for the detection of multi-class pharmaceutical micropollutants in water matrices. The study encompasses comprehensive spectral characteristic of the selected active substance from the band assignment to the systematic investigation of pH-dependent changes. The quantitative potential of the approach is evaluated through calibration experiments aimed at establishing limits of detection relevant to environmentally occurring concentration levels.

The presented work demonstrates the versatility of SERS for addressing the analytical complexity arising from structurally diverse pharmaceutical contaminants, and discusses its potential as a complementary tool in environmental water quality monitoring.

Keywords: Surface-Enhanced Raman Spectroscopy, Pharmaceutical Micropollutants, Silver nanostructures, Emerging contaminants

Posters

[Abstract:0528] [SERS/TERS/Plasmonics]

Surface-Enhanced Raman Spectroscopy in Multi-Omics Integration for Melanoma Profiling

***David Lilek*[1], *Anna Mayr*[1], *Magdalena Hohlrieder*[1], *Isabella Pauser*[1], *Agnes Grünfelder*[1], *Justyna Rechthaler*[1], *Sonja Gamsjaeger*[3], *Bodo D. Wilts*[2], *Maurizio Musso*[2], *Christoph Wiesner*[4], *Birgit Herbinger*[1], *Katerina Prohaska*[1]**

[1]*Biotech Campus Tulln, University of Applied Sciences Wiener Neustadt, Austria*
[2]*Department of Chemistry and Physics of Materials, Paris Lodron University Salzburg, Austria*
[3]*Ludwig Boltzmann Institute of Osteology at the Hanusch Hospital of OEGK and AUVA Trauma Centre Meidling, Vienna, Austria*
[4]*Institute Biotechnology, IMC Krems University of Applied Sciences, Krems an der Donau, Austria*

Melanoma is an aggressive skin cancer in which reliable diagnosis at early stage is critical for patient outcome. Understanding the transition from non-metastatic to metastatic stages requires detailed characterization of molecular and phenotypic differences. In this study, we investigated non-metastatic (MCM-1G) and metastatic (MCM-DLN) melanoma cell lines. A key challenge in Raman-based diagnostics is the validation and biological interpretation of spectral data, which we aim to address by automatized correlation with complementary transcriptome and proteome datasets.

Transcriptomic analysis by RNA-seq revealed 8,451 differentially expressed genes, with the most prominent changes including upregulation of ribosome biogenesis and translational machinery, and downregulation of ECM organization, cell adhesion molecules and immune processes in MCM-DLN, consistent with a pro-invasive and immunoevasive phenotype[AG1.1]. Bottom-up proteomics using an HR-MS/MS system identified 37 significantly regulated proteins, highlighting functional divergence between both cell lines. Proteins such as NOL3 and RALBP1 were upregulated in MCM-DLN, supporting tumour progression, whereas MOB1B was elevated in MCM-1G, consistent with tumour-suppressive functions. Additional markers, including GNMPB and CD151, reflect differences in melanin production and cell–cell communication.

For SERS analysis, we employed a self-assembled solid substrate based on gold nanoparticles and acquired spectra using a Raman microscope (Senterra I - 785nm laser). This approach yielded highly reproducible results across both biological and technical replicates. For data analysis, several supervised machine learning methods were applied, with logistic regression using L1 regularization achieving the best performance (AUC = 0.9876). For MCM-1G, sparse model coefficients identified key features at 965 and 1250 cm^{-1}, corresponding to lipid-associated CH_3 deformation and amide III changes. In contrast, MCM-DLN exhibited dominant features at 650, 1001, 1219, and 1614 cm^{-1} attributed to protein vibrations (e.g., tyrosine, pyrimidine, amide III, tryptophan). These findings demonstrate that metastatic progression can be reliably distinguished by SERS.

Overall, the integration of transcriptomics, proteomics, and SERS provides a coherent multi-omics framework linking molecular alterations to spectral signatures. This approach strengthens the interpretability and robustness of label-free diagnostics. Future work will focus on automating multi-omics integration, and validating these findings in more complex clinical samples, with the aim of translating SERS-based diagnostics into routine clinical decision-making.

Keywords: SERS, melanoma, multi-omics, transcriptomics, proteomics, machine learning

[Abstract:0530] [Biology/Biomedicine]

High-Throughput Raman-Activated Cell Sorting (HT-RACS) Using Acoustofluidic Chip with Elasto-Inertial Focusing

***Gyeong Tae Kim*[1], *Gwanghyeon Yu*[2], *Jeongeun Park*[3], *Hyun Uk Kim*[3], *Jin Ho Yun*[4], *Jinsoo Park*[3], *Sung Chul Bae*[1], *Kang Soo Lee*[2]**

[1]*Department of Biomedical Engineering, Ulsan National Institute of Science and Technology (UNIST), Ulsan, Republic of Korea*
[2]*Department of Mechanical Engineering, Ulsan National Institute of Science and Technology (UNIST), Ulsan, Republic of Korea*
[3]Department of Mechanical Engineering, Chonnam National University, Gwangju, Republic of Korea
[4]*Cell Factory Research Center, Korea Research Institute of Bioscience & Biotechnology (KRIBB), Daejeon, Republic of Korea*

Resolving cellular heterogeneity at single-cell resolution and linking phenotypes to genotypes remain central challenges in microbial research, particularly for elucidating the metabolic mechanisms of individual cells. Raman-activated cell sorting (RACS) offers a compelling label-free solution by leveraging intrinsic molecular fingerprints. However, existing implementations are constrained by a fundamental trade-off between spectral signal-to-noise ratio (SNR) and sorting throughput, limiting their practical utility.

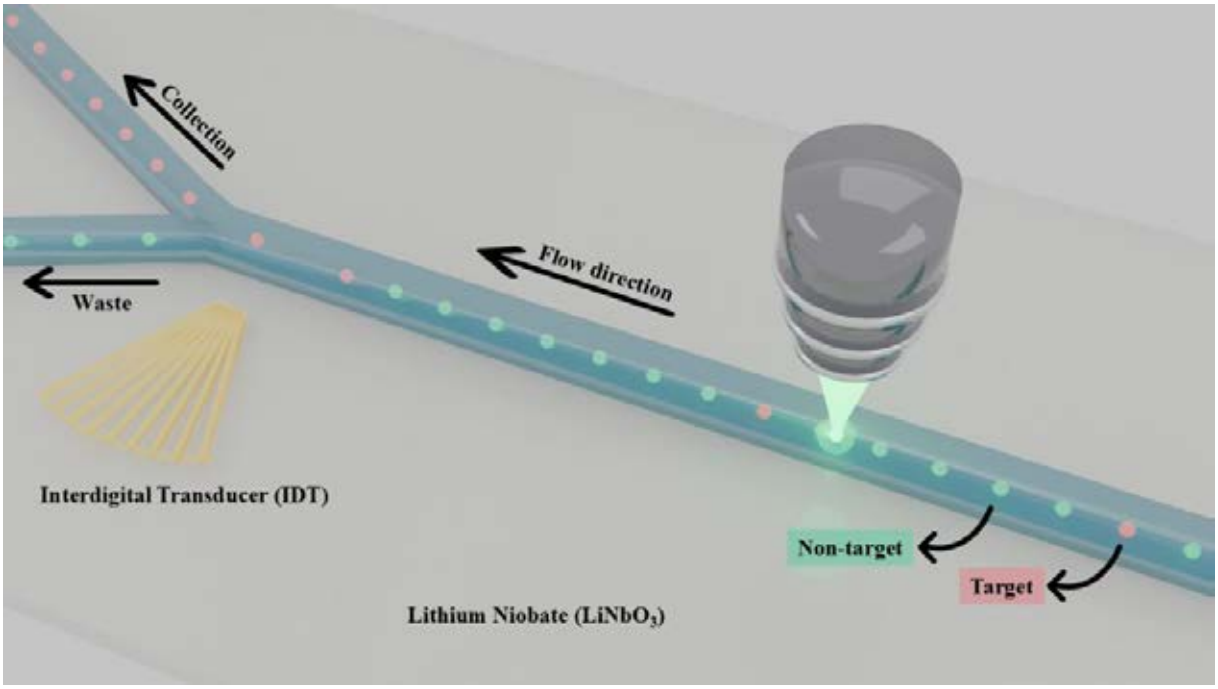
Here, we present a high-throughput RACS (HT-RACS) platform that integrates confocal Raman microspectroscopy with a lithium niobate ($LiNbO_3$) acoustofluidic chip featuring poly(ethylene oxide) (PEO)-based elasto-inertial 3D focusing and traveling surface acoustic wave (TSAW) actuation for the sorting of target cells. Three-dimensional, single-file cell focusing is achieved through viscoelastic normal stress in a microfluidic channel, ensuring deterministic cell positioning within the confocal Raman interrogation volume. Center-aligned samples flowing at controlled velocity undergo on-the-fly Raman-based classification, and those identified as targets are selectively deflected at the sorting junction via TSAW.

The performance of the proposed system is experimentally validated through a two-stage demonstration. First, polystyrene (PS) and poly(methyl methacrylate) (PMMA) microparticles, which exhibit distinct Raman spectral signatures (e.g., aromatic ring breathing at ~1,001 cm^{-1} for PS and ester carbonyl stretching at ~1,730 cm^{-1} for PMMA), are employed as a well-characterized binary mixture to verify the accuracy and reliability of Raman-based detection within the 3D focusing geometry and TSAW-driven sorting mechanism. Subsequently, the system is applied to the selective sorting of *Chlorella* microalgae based on their photosynthetic efficiency — an important biochemical phenotype for biotechnological applications — demonstrating the capability to isolate cells exhibiting favorable intracellular compositions from a heterogeneous population in a label-free manner.

These results establish the HT-RACS platform as a high-throughput, label-free single-cell sorting system whose compact architecture and straightforward operational workflow enable accessible and rapid adoption across diverse disciplines, including biofuel development, environmental monitoring, and biomedical diagnostics.

Keywords: Raman-activated cell sorting, acoustofluidics, elasto-inertial focusing, confocal Raman microspectroscopy

Scheme of the HT-RACS system



Posters

[Abstract:0533] [Coherent Raman Imaging]

From Glass Slides to Water Filters: Broadband SRS Workflow for Microplastics Identification

***Federica Padelli*[1], *Eric Michele Fantuzzi*[2], *Eleonora Erriquez*[2], *Rebeca Martinez Vazquez*[4], *Alessandra Nardini*[1], *Matteo Corti*[2], *Gabriele Di Noia*[2], *Mujeeb Rahman*[3], *Federico Monti*[2], *Andrea Ragni*[2], *Giulio Nicola Felice Cerullo*[1], *Francesco Crisafi*[2]**

[1]*Politecnico di Milano, Dipartimento di Fisica, P.zza Leonardo da Vinci 32, 20133, Milan, Italy*
[2]*Cambridge Raman Imaging Srl, Via Durando 39, 20158, Milan, Italy*
[3]*Cambridge Raman Imaging Ltd, Botanic House, 100 Hills Road, Cambridge, Cambridgeshire, CB2 1PH, United Kingdom*
[4]*Consiglio Nazionale delle Ricerche (CNR), Istituto di Fotonica e Nanotecnologie (IFN), Piazza Leonardo da Vinci 32, 20133, Milan, Italy*

Microplastics pollution is becoming a global environmental and health concern, driving the need for analytical tools capable of fast, reliable, and high-resolution detection, identification, and quantification. Conventional techniques, such as Fourier-transform infrared (FTIR) spectroscopy, spontaneous Raman microscopy, scanning electron microscopy (SEM), and pyrolysis–gas chromatography–mass spectrometry (Py-GC/MS), are widely adopted for microplastics analysis. However, their broader implementation is limited by spatial resolution, long acquisition times, laborious sample preparation, high operational costs, and the potential for contamination or sample degradation.

To address these limitations, we developed CORAL, an advanced imaging platform based on broadband Stimulated Raman Scattering (SRS) microscopy, developed at Cambridge Raman Imaging for rapid and label-free microplastics analysis. CORAL enables the simultaneous acquisition of 38 spectral channels across the C–H stretching region (2800–3100 cm^{-1}) within a few microseconds, combining chemical specificity, high spatial resolution, and speed in a single modality.

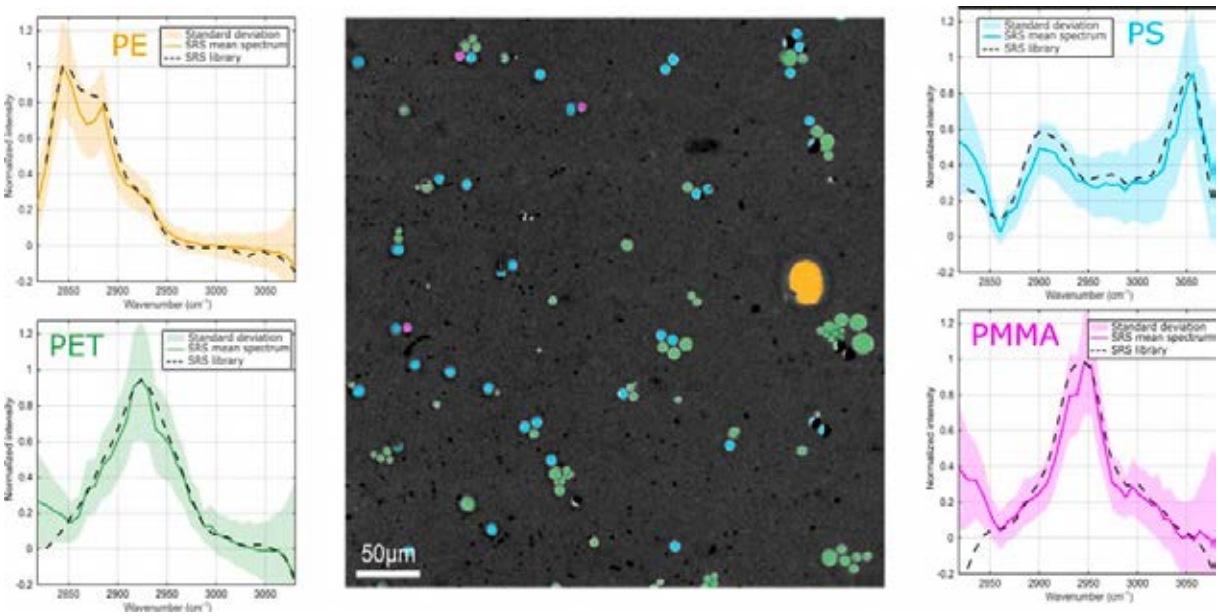
In this work, we demonstrate the capability of CORAL to identify and discriminate microplastics across different substrates and experimental configurations. A spectral library was established using particles with diverse polymer compositions, morphologies, and sizes. Measurements were performed on particles deposited on glass slides and on membrane filters commonly employed in environmental collection workflows, confirming the robustness of the approach under conditions relevant to real-world analysis.

In addition, we show the in-flow detection and identification of microplastics in aqueous systems using custom-designed silica flow cells. The simultaneous acquisition of the full C–H spectral window enables the investigation of dynamic processes that are challenging for conventional Raman-based or sequential SRS approaches. This feature opens new opportunities for real-time monitoring of microplastics in fluidic environments.

Overall, our results position broadband SRS microscopy as a powerful alternative for fast, label-free microplastics characterization, with strong potential for extension to complex matrices, including biological tissues.

Keywords: Microplastics, Stimulated Raman Scattering (SRS), Broadband SRS Microscopy, In-flow Detection, filters

Pearson's correlation-based overlay of PE, PS, PET and PMMA



Pearson's correlation-based overlay of the four microplastic types: Polyethylene (PE), Polystyrene (PS), Polyethylene terephthalate (PET) and Polymethyl Methacrylate (PMMA) identified on an alumina filter. For each class, the mean spectrum of the classified pixels is reported together with the associated standard deviation and the corresponding reference spectrum from SRS library.

[Abstract:0536] [Novel Approaches]

Toward Single-Particle Raman Microscopy of Vitrified Biological Samples at Liquid Helium Temperature

***Polina Kasyanova*, Hisham Mazal, Vahid Sandoghdar**

Max Planck Institute for the Science of Light, 91058 Erlangen, Germany

Raman imaging is highly attractive for biological research because it provides rich molecular information in a label-free manner. However, due to its intrinsically small scattering cross section, the signal-to-noise ratio in Raman measurements is severely limited. Consequently, biological samples often require illumination at high laser powers or long acquisition times to obtain a usable signal. Recent advances have shown that combining cryofixation with low-temperature Raman imaging can overcome these limitations. In particular, cryogenic conditions reduce diffusion artifacts and allow for longer acquisition times without inducing substantial cellular damage. This approach was recently realized using a cooling stage mounted on a room-temperature microscope, enabling freeze-drying and imaging of samples at liquid nitrogen temperature (77 K). However, the relatively slow freezing process, along with the need for continuous nitrogen gas flow to minimize ice condensation, makes this method suboptimal, compromising sample integrity and introducing mechanical and thermal drift. To fully harness the advantages of cryogenic Raman imaging of biological samples, we take advantage of shock freezing. Here, we use a custom-built high-vacuum cryogenic shuttle system that enables controlled transfer into and out of a cryogenic microscope operating at liquid helium temperature (4 K). We recently used this system for super-resolution fluorescence microscopy with angstrom precision. In this presentation, we discuss our Raman studies on simple biological specimen maintained in vitreous ice. Our approach paves the way toward high-sensitivity, single-particle cryogenic Raman imaging of vitrified biological systems, with the potential to reveal previously inaccessible biochemical information.

Keywords: Cryogenic Raman imaging, shock-freezing, vitrification, single-particle analysis

[Abstract:0537] [Novel Approaches]

From Raman Spectrometers to Sensors: A New Architecture for High-Resolution Raman Detection

***Oliver Lischtschenko*[1], *Katarzyna Szykuła Meurs*[2]**

[1]*Coher Sense UG, Lübeck, Germany*
[2]*M4i Institute in the Faculty Health, Medicine & Life Sciences, Maastricht University, Maastricht, The Netherlands*

In this work, we present a novel Raman sensing architecture based on polarization-interferometry. Instead of acquiring a complete Raman spectrum, the proposed approach selectively targets Raman bands of interest using optical filters and measures their position with picometer-scale resolution. By focusing on individual Raman features rather than the entire spectrum, the system achieves wavelength accuracy far beyond that of conventional Raman spectrometers, while operating at measurement rates extending into the MHz regime.

The concept is particularly suited for applications where changes in a specific Raman vibration contain the relevant process information. Examples include monitoring temperature-induced peak shifts, detecting contamination, tracking reaction progress, or observing phase transitions. In these cases, acquiring a full Raman spectrum may not be necessary once the relevant spectral feature has been identified.

The presented architecture combines fixed optical filters with an interferometric wavelength sensor. This sensor-based approach significantly reduces system complexity while enabling precise tracking of Raman peak positions and spectral shifts. Unlike traditional Raman workflows, which often rely on multivariate analysis and chemometric models to extract process information from large spectral datasets, the proposed method directly measures the parameter of interest, simplifying both instrumentation and data analysis. The proposed architecture is not intended to replace conventional Raman spectroscopy, but rather to complement it by enabling compact, fast, and highly sensitive Raman sensors optimized for wavelength shifts. Such systems may provide a promising route toward broader deployment of Raman technology in process analytical technology (PAT), industrial monitoring and application-specific sensing.

Keywords: Raman, Optics, Interferometry, Polarisation, PAT, Instrumentation

[Abstract:0540] [Biology/Biomedicine]

Monitoring Brain Tumors by Non-invasive, Label-free Surface-Enhanced Raman Spectroscopy on Biofluids

***Salomé Thueler*[1], *Johanna Joyce*[3], *Andreas Hottinger*[5], *Sabine Galland*[4], *Christophe Galland*[2]**

[1]*School of Life Sciences, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*
[2]*Institute of Physics, Laboratory of Quantum and Nano Optics, École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*
[3]*Professor Joyce Laboratory, Agora Cancer Research Centre Lausanne, Switzerland*
[4]*Ludwig Institute for Cancer Research, University of Lausanne, Lausanne, Switzerland*
[5]*Lundin Family Brain Tumor Research Center, CHUV, Lausanne, Switzerland*

Glioblastomas are aggressive forms of brain tumors, with a median progression-free survival time of approximately 7 months, eliciting the need to improve patient care by close monitoring of disease progression. Current post-surgical follow-up relies on MRI scans performed at relatively long intervals, which may impair the early detection of relapse.

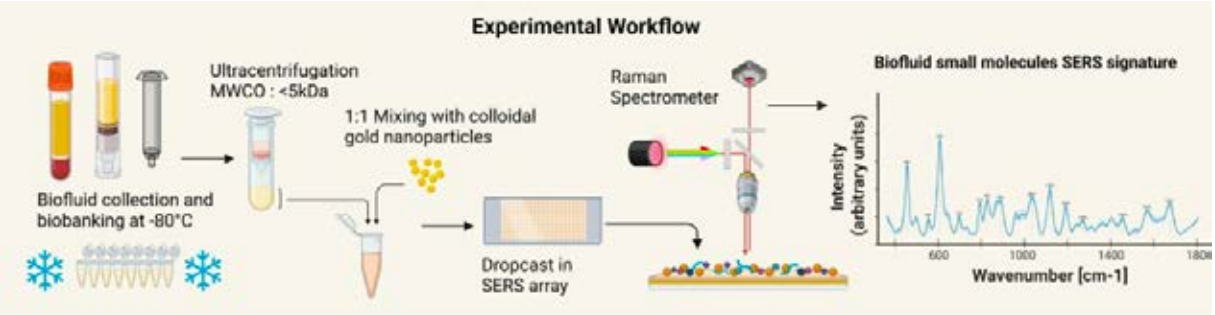
Surface-Enhanced Raman Spectroscopy (SERS) provides molecular fingerprints that reflect the unique chemical composition of biological samples through inelastic photon scattering, locally amplified by electromagnetic field–enhancing gold nanoparticles. Applied to biofluids such as serum, plasma, saliva or urine, SERS offers a fast, low-cost, straightforward, and highly sensitive analytical approach, making it a promising candidate for the development of a routine liquid biopsy.

In this project we aim to integrate longitudinal SERS profiling of blood plasma with relevant clinical data from patients with glioblastoma, low-grade brain tumors, or brain metastases, alongside a healthy donor cohort. Multivariate statistical analyses and machine learning approaches will be used to identify spectral fingerprints and temporal patterns associated with early disease recurrence. These findings will be correlated with MRI-based tumor monitoring and standard blood analysis, including serum chemistry and hormone levels

The poster presents early work supporting this research goal. We provide an in-depth investigation of nanoparticle-blood plasma interactions, assessing the impact of gold nanoparticle properties, including size, shape, manufacturer, concentration, and incubation ratio, as well as plasma pre-processing by ultracentrifugation on SERS spectra. We focus particularly on uric acid, a major Raman-active component of blood plasma, and demonstrate how variations in the uric acid-to-nanoparticle ratio influence spectral features. Additionally, we introduce a straightforward fabrication method for multi-well gold-mirror slides, enabling multiplexed analysis of up to 50 samples per slide. Finally, we demonstrate the repeatability and robustness of our sample preparation protocol across operators and substrates, evaluate substrate stability over time, and provide initial insights into inter- and intra-donor spectral variability in both healthy donors and patients with resected brain tumors.

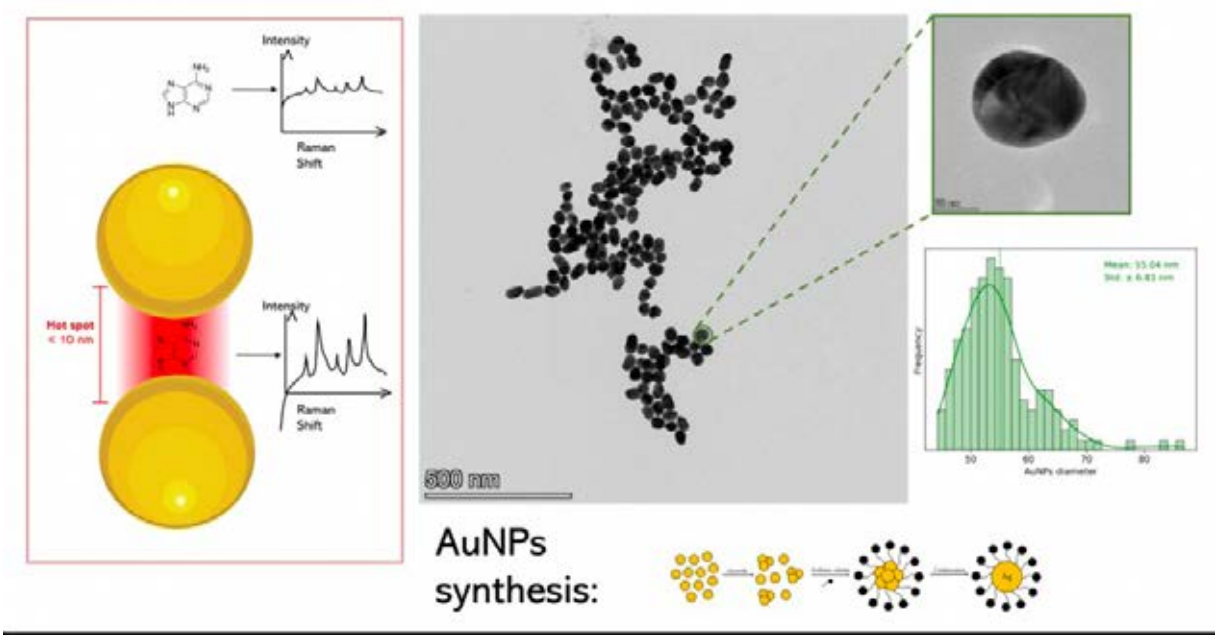
Keywords: SERS, biosensing, blood, glioblastoma, nanoparticle, liquid biopsy

SERS-based molecular fingerprinting of blood-derived biofluids



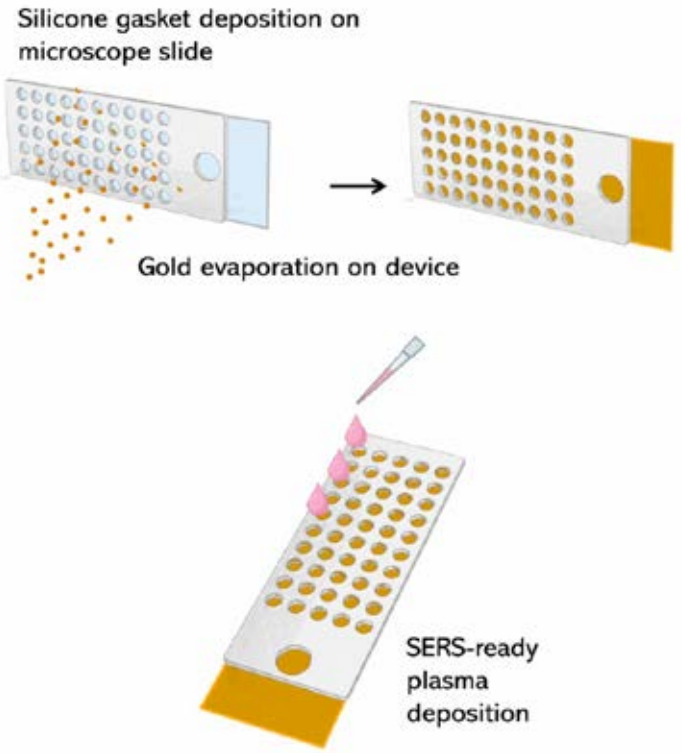
Early detection of brain tumor recurrence is critical for improving patient outcomes. Brain tumors include brain metastases (BrM) and primary tumors, with glioblastoma (GBM) being the most aggressive form, showing median progression-free survival of ~7 months and overall survival under two years. Standard follow-up via MRI can miss early relapse due to post-treatment tissue changes, underscoring the need for more sensitive monitoring approaches. We explore Surface Enhanced Raman Spectroscopy (SERS), a rapid, non-invasive, label-free optical technique, to detect molecular signatures of early relapse or treatment response in patient blood. We longitudinally monitor SERS spectra from patient blood collected pre and post-surgery and during follow-up, correlating findings with clinical and radiological data. Integrating multivariate statistics and machine learning, we aim to identify spectral fingerprints predictive of early relapse or treatment response, supporting the development of routine liquid biopsies.

Gold nanoparticle synthesis & characterization



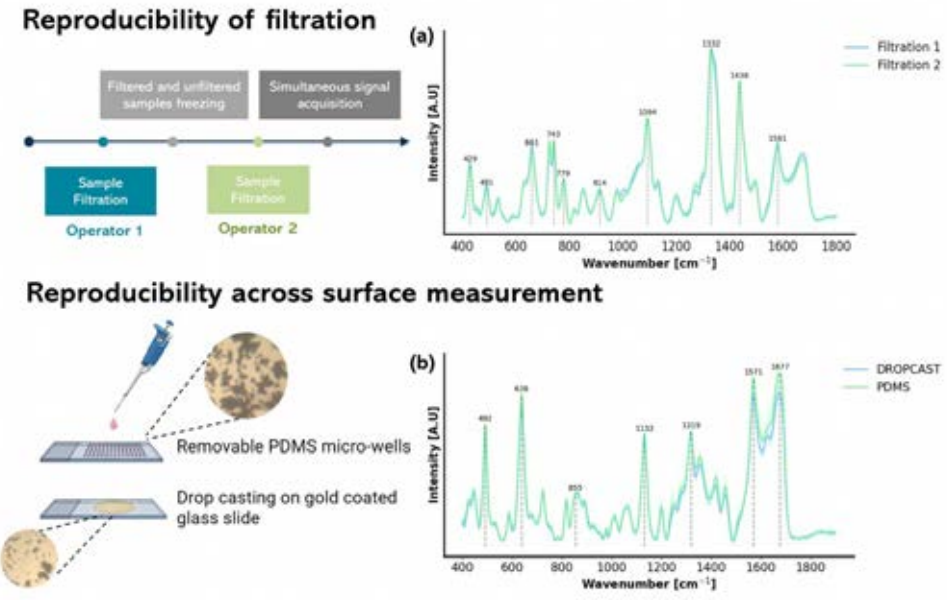
Gold nanoparticle: Spherical gold nanoparticles were synthesized and characterized using UV-Vis spectroscopy and TEM. To reduce signal background from high molecular weight organic components, human serum and plasma samples were prepared using ultrafiltration or size-exclusion chromatography. Gold nanoparticles were concentrated and mixed with the biofluids, then drop-cast onto gold-coated surfaces, or dispensed in PDMS-microwells.

Microwells on gold mirror for high-throughput SERS acquisitions



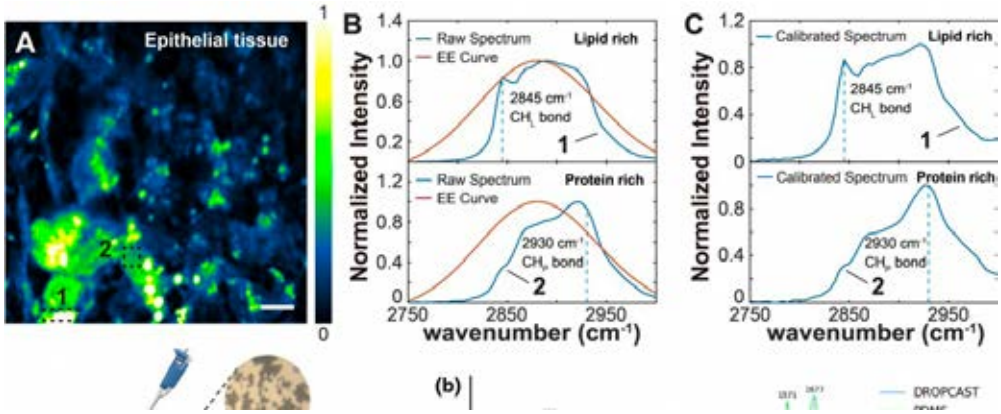
Design of a simple Improved nanoparticle aggregation Compatible with automatized sample acquisition Flexible design, extendable to larger arrays

Reproducibility of SERS spectra across filtrations and substrates on GBM patient plasma (a) and commercial human serum (b)



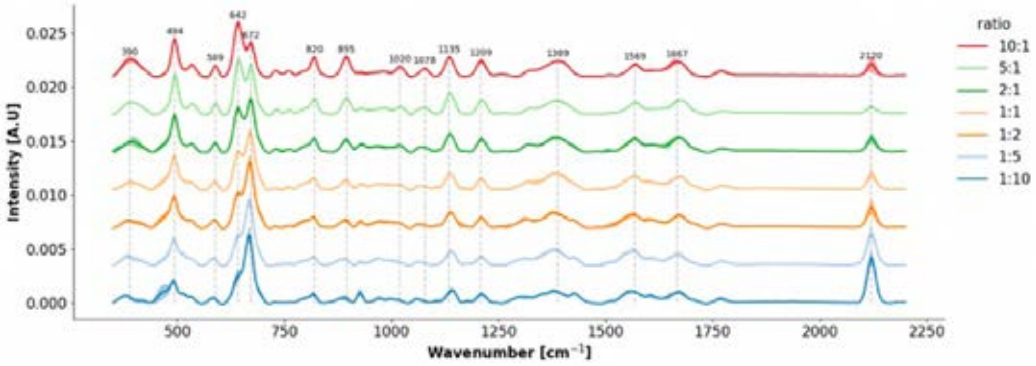
Blood plasma samples prepared by ultracentrifugation (MWCO < 5kDa) by two operators show the reproducibility of the obtained SERS spectra. Using PDMS or silicone gasket enable controlled dispense of sample on gold mirror without introducing a bias in the measure spectra.

Impact of nanoparticle shape on serum SERS spectra



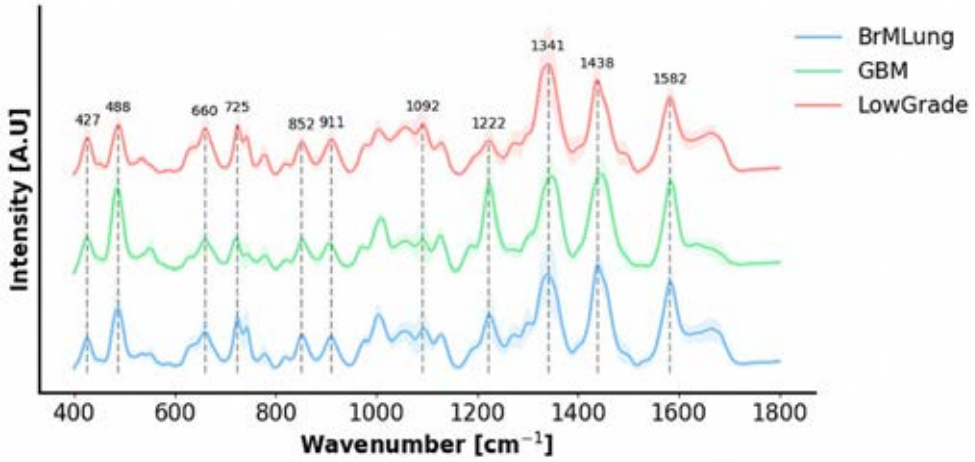
Spectra acquired on mice filtered serum using spherical (55nm), decahedral (38nm) or nanostars-shaped nanoparticle highlight the influence of the nanoparticle shape on the detectable spectral features.

Uric acid spectra variation along with nanoparticle:uric acid ratio

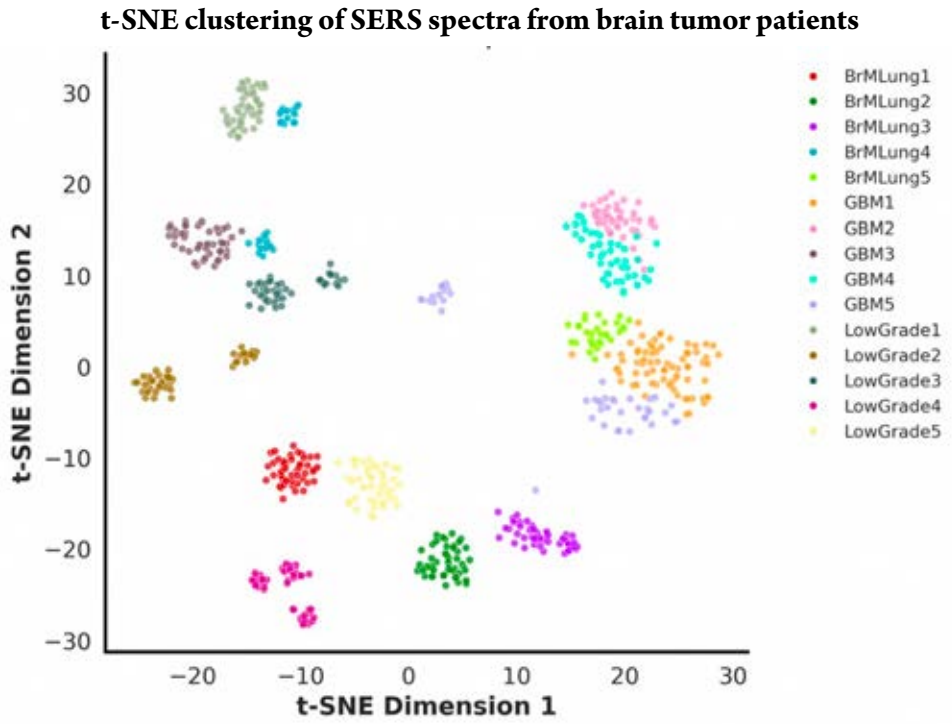


Uric acid (350uM in PBS) is mixed at different volume ratio with colloidal gold nanoparticles (OD5). We observe that features at 642cm-1 and 672 cm-1 are varying along with the changes of nanoparticles to uric acid ratio.

Average SERS spectra per brain tumor subtype



Representation of average spectra per group, n=5 patients per group, 30-45 spectra per patient



Dimensionality reduction (t-SNE) of SERS plasma samples from BrM, GBM and LowGrade brain tumor show patient-dependant clustering.

Posters

[Abstract:0541] [SERS/TERS/Plasmonics]

Dielectrophoretic Trapping and SERS-Based Detection of Micro- and Nanoplastics in Water

***Tomasz Szymborski*[1], *Adam Samborski*[1], *Aneta A Kowalska*[1], *Sławomir Błoński*[2], *Piotr Korczyk*[2], *Agnieszka Kamińska*[1]**

[1]*Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland*
[2]*Institute of Fundamental Technological Research, Polish Academy of Sciences, Warsaw, Poland*

Contamination of aquatic environments with micro- and nanoplastics is a growing environmental and analytical challenge. Particular concern is associated with their presence in drinking water, where small plastic particles may occur at low concentrations, exhibit broad size distributions (from the nanometre scale to several hundred micrometres) and coexist with complex inorganic and organic matrix components. Reliable detection and identification of micro- and nanoplastics in water remain challenging because conventional analytical workflows often require laborious sample preparation, particle preconcentration (e.g. by filtration, hydrocyclone-based or density-based separation) and subsequent spectroscopic or microscopic characterization.

We present an integrated approach for the detection of micro- and nanoplastics in water based on the combination of microfluidic particle handling, dielectrophoretic (DEP) trapping and surface-enhanced Raman spectroscopy (SERS). The proposed approach uses non-uniform electric fields generated in a microfluidic system to manipulate and concentrate plastic particles in a defined detection region. Dielectrophoresis offers a label-free mechanism for particle trapping that depends on the dielectric properties of the particles and the surrounding medium, and may therefore support selective enrichment of micro- and nanoplastics from aqueous samples. The trapped particles can be analysed directly via SERS, which provides molecularly specific vibrational information and enhanced Raman sensitivity through interaction with a plasmonic SERS-active substrate.

Combining dielectrophoretic trapping with SERS detection is intended to address two key limitations in micro- and nanoplastic analysis: the low number of particles available in small sample volumes and the difficulty of obtaining sufficiently strong and characteristic Raman signals from individual or weakly accumulated particles. A microfluidic implementation may additionally improve control over sample volume, particle transport, trapping location and measurement reproducibility.

Keywords: SERS, microplastics, nanoplastics, dielectrophoresis, microfluidics

[Abstract:0542] [SERS/TERS/Plasmonics]

Advanced Engineering of AuNP-on-AuNF Junctions for Highly Reproducible and Sensitive Induced Surface-Enhanced Raman Optical Activity (SEROA)

***Woongil Jeon*, Daehong Jeong**

Department of Chemistry Education, Seoul National University, Seoul, Republic of Korea

Surface-enhanced Raman optical activity (SEROA) offers a sophisticated pathway for chiral discrimination, yet its practical application has been hindered by the lack of reproducible substrates at the single-hotspot level. This study presents an advanced development of the Gold Nanoparticle-on-Gold Nanofilm (AuNP-on-AuNF) architecture, focusing on the rigorous control of substrate uniformity to achieve a significantly enhanced limit of detection (LOD). Building on previous findings that established the AuNP-on-AuNF junction as a superior platform for confining electromagnetic fields and minimizing circular dichroism (CD) interference, we have further refined the fabrication process to suppress inter-particle variability.

By achieving precise, uniform control over the nanoparticle distribution and junction geometry, we have minimized the signal fluctuations that typically plague SERS-based chiral measurements. This structural optimization, combined with an optimized 532 nm excitation allows for the acquisition of highly consistent and reproducible induced-SEROA spectra. The improved statistical reliability of the data enables a more precise analytical transition from qualitative chiral sensing to quantitative ultra-trace detection. Consequently, this advanced platform demonstrates a superior LOD and enhanced enantiomeric discrimination capabilities compared to earlier models. This work underscores the critical importance of single-particle level substrate engineering in transitioning SEROA into a robust, high-performance diagnostic technology.

Keywords: AuNP-on-AuNF Junction, Surface-Enhanced Raman Optical Activity (SEROA), Inter-particle Variation, Chiral Sensing

[Abstract:0544] [Coherent Raman Imaging]

Data-Driven Selection of Raman Signatures for Label-Free SRS Imaging of Lipid Metabolism in HER2-Positive Breast Cancer

***Tamás Váczi*[1], *Péter Áron Tóth*[2], *Dorottya Vígh*[2], *Miklós Veres*[1], *László Virág*[2], *István Csarnovics*[3], *Endre Kókai*[2], *Endre Kókai*[4]**

[1]*Department of Photonics, Institute of Solid State Physics and Optics, HUN-REN Wigner Research Centre for Physics, Budapest, Hungary*
[2]*Department of Medical Chemistry, Faculty of Medicine, University of Debrecen, Debrecen, Hungary*
[3]*Department of Experimental Physics, Institute of Physics, Faculty of Science and Technology, University of Debrecen, Debrecen, Hungary*
[4]*Section of Dental Biochemistry, Department of Basic Medical Sciences, Faculty of Dentistry, University of Debrecen, H-4032 Debrecen, Hungary*

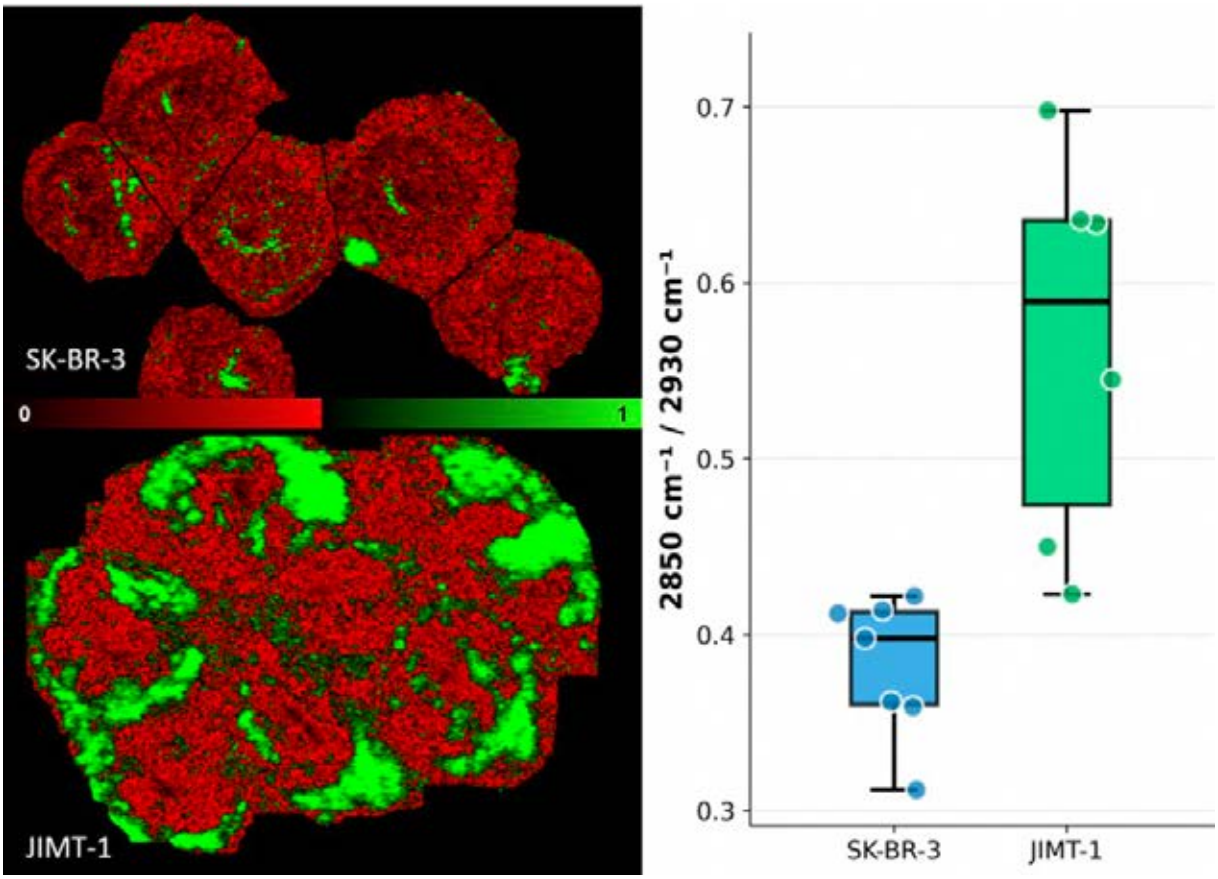
Distinguishing functionally distinct cancer cell lines through non-invasive means is a critical goal in cancer biology. In this study, we applied a label-free vibrational spectroscopy framework to investigate two HER2-positive breast cancer cell lines with differing trastuzumab sensitivity: JIMT-1 (resistant) and SK-BR-3 (sensitive).

Instead of targeting predefined characteristic molecular vibrational signatures, we utilized spontaneous Raman microspectroscopy combined with machine learning to identify the dominant biochemical axes of variation between these lines. A PCA-SVM classifier achieved 96% accuracy (AUC 0.99) in the fingerprint region (1050–1790 cm^{-1}). To identify the biochemical discriminants underlying this classification, we performed permutation importance analysis, projecting importance scores back onto the wavenumber axis. This unbiased approach identified lipid-associated vibrations, specifically C–H deformation (1437 cm^{-1}) and C–C skeletal stretching (1062 cm^{-1}), among the primary discriminants in the fingerprint region. Analysis of the high-wavenumber region (2800–3100 cm^{-1}) reinforced this, with the most informative features being the CH_2 symmetric stretch (2850 cm^{-1}) and the CH_2 antisymmetric stretch (2883 cm^{-1}).

These results directly informed our stimulated Raman scattering (SRS) imaging strategy. Using the identified signatures, we performed ratiometric SRS imaging at 2850 cm^{-1} and 2930 cm^{-1}, highlighting cellular lipid-to-protein content, to orthogonally validate the lipid-associated spectral differences with subcellular resolution. Ratiometric SRS maps revealed a significantly elevated lipid-to-protein ratio in JIMT-1 cells compared to SK-BR-3 (mean 0.564 vs. 0.383, respectively), confirming an inherently more lipid-rich phenotype in the resistant line (Figure 1). Quantified across imaging fields, these lipid-rich structures were prominently distributed throughout the JIMT-1 cytoplasm, whereas SK-BR-3 displayed a protein-dominated profile. This higher lipid burden was further associated with a selective, concentration-dependent sensitivity to hemin-induced lipid peroxidation in JIMT-1. Our findings demonstrate that Raman-based feature selection combined with SRS imaging provides a powerful, label-free discovery tool for identifying functionally relevant metabolic biomarkers in cancer cells.

Keywords: label free, SRS, lipid metabolism, chemometrics

Figure 1



Left: SK-BR-3 and JIMT-1 cells, showing differences in lipid distribution patterns based on ratiometric analysis of SRS images (2850 cm^{-1}/2930 cm^{-1}). Right: Plot of measured lipid-to-protein ratios per imaging field.

Posters

[Abstract:0547] [SERS/TERS/Plasmonics]

Antibody-Functionalized Fe_3O_4@Au Magnetoplasmonic Nanoparticles for SERS-Based Bacterial Detection

***Rumeysa Polat*[1], *Münevver Akdeniz*[1], *Omer Aydin*[2]**

[1]*Department of Biomedical Engineering, Erciyes University, Kayseri, Türkiye, NanoThera Lab, Drug Application and Research Center (ERFARMA), Erciyes University, Kayseri, Türkiye*
[2]*Department of Biomedical Engineering, Erciyes University, Kayseri, Türkiye, NanoThera Lab, Drug Application and Research Center (ERFARMA), Erciyes University, Kayseri, Türkiye, Clinical Engineering Research and Implementation Center (ERKAM), ErciyesUniversity, Kayseri, Türkiye, Nanotechnology Research and Application Center (ERNAM), Erciyes University, Kayseri, Türkiye, Betul Ziya Eren Genome and Stem Cell Center (GENKOK), Erciyes University, Kayseri, Turkey*

Rapid and sensitive detection of pathogenic bacteria is essential for food safety, environmental monitoring, and clinical diagnostics. However, conventional bacterial detection methods are often time-consuming and require labor-intensive procedures. In this study, a magnetoplasmonic surface-enhanced Raman spectroscopy (SERS) platform based on Fe_3O_4@Au core–shell nanoparticles is being developed for the selective detection of bacteria.

Fe_3O_4@Au nanoparticles were functionalized with 4-mercaptobenzoic acid (4-MBA) as a Raman reporter molecule through Au–S interactions. The carboxyl groups of 4-MBA will subsequently be activated using EDC/NHS chemistry to enable covalent conjugation of specific antibodies onto the nanoparticle surface. The resulting immuno-functionalized nanoprobes are expected to provide selective recognition and capture of target bacteria. The Fe_3O_4 magnetic core enables rapid magnetic separation and enrichment, while the Au shell generates localized surface plasmon resonance, facilitating enhanced Raman signal amplification.

At the current stage of the study, the nanoparticles were characterized using zeta potential analysis, UV–Vis spectroscopy, dynamic light scattering (DLS), nanoparticle tracking analysis (NTA), and scanning transmission electron microscopy (STEM). The UV–Vis absorption spectrum of the Fe_3O_4@Au nanoparticles exhibited a characteristic peak at 560 nm, confirming the successful formation of the gold shell, whereas Fe_3O_4 nanoparticles showed no significant absorption peak. Following immobilization of the Raman reporter molecule, a red-shift in the plasmonic absorption peak was observed, indicating successful surface modification. In addition, Raman measurements confirmed the immobilization of 4-MBA through its characteristic vibrational bands at 1078 cm^{-1} and 1588 cm^{-1}.

In the next stage of the study, antibody conjugation and bacterial sensing experiments will be performed. When interacting with target bacteria, the formation of nanoparticle–bacteria complexes is expected to induce measurable changes in SERS intensity, enabling sensitive bacterial detection. The proposed sensing strategy integrates magnetic enrichment, antibody-based selective targeting, and SERS detection within a single nanoplatform. These findings highlight the potential of Fe_3O_4@Au–4MBA nanoparticles as a promising platform for rapid and sensitive bacterial detection and future point-of-care diagnostic applications.

Keywords: Surface-enhanced Raman spectroscopy, Fe3O4@Au nanoparticles, bacterial detection, antibody conjugation, magnetoplasmonic biosensor

[Abstract:0554] [Novel Approaches]

Correlative Multimodal Vibrational Imaging with Integrated O-PTIR and PT-SRS for High-Speed Label-Free Chemical Analysis

***Miriam Unger*[1], *Mustafa Kansiz*[2], *Yuhao Yuan*[2], *Craig Prater*[2]**

[1]*Photothermal Spectroscopy Corp. GmbH, Muelheim, Germany*
[2]*Photothermal Spectroscopy Corp., Santa Barbara, CA, United Stated*

High-resolution chemical imaging of heterogeneous samples often requires balancing spatial resolution, imaging speed, and molecular specificity, particularly in label-free biological and materials analysis. To address these challenges, we present an integrated multimodal imaging platform that combines Optical Photothermal Infrared (O-PTIR) spectroscopy and Photothermal Stimulated Raman Scattering (PT-SRS; also referred to as Stimulated Raman Photothermal, SRP) within a unified laser-scanning microscope for real-time, label-free vibrational imaging.

The combined O-PTIR/PT-SRS workflow enables submicron chemical imaging by leveraging complementary infrared and Raman vibrational contrast within a unified platform. High-speed synchronized beam scanning supports rapid acquisition of large-area hyperspectral datasets while maintaining spatial detail at the subcellular scale. In addition to planar imaging, depth-resolved measurements enable three-dimensional chemical characterization of complex specimens. Adaptable optical configurations, including co-propagating and counter-propagating geometries, extend compatibility across a broad range of sample environments, including both IR-transparent and IR-opaque substrates.

To support correlative workflows, the instrument incorporates multi-line widefield fluorescence together with laser-scanning confocal fluorescence microscopy, enabling targeted localization of regions of interest prior to vibrational analysis. Applications spanning both life and materials sciences are demonstrated through representative measurements of polymer mixtures, microplastic distributions, brain tissue sections, and dynamic lipid-rich subcellular structures in live cells. These examples highlight the platform's ability to deliver chemically specific, label-free imaging across diverse sample types while maintaining throughput suitable for large-area analysis.

The integration of O-PTIR, PT-SRS, and fluorescence modalities within a single system establishes a versatile framework for multimodal chemical imaging with applications spanning biological research, environmental analysis, and advanced materials characterization.

Keywords: O-PTIR, PT-SRS, Chemical Imaging

Posters

[Abstract:0559] [Materials]

Evaluating Picolinamide as a Cocrystal Former with Acidic Coformers

***Ainur Syeitkhajy*[1], *Neris Inci Inan*[1], *Gulce Ogruc Ildiz*[2], *Rui Fausto*[3]**

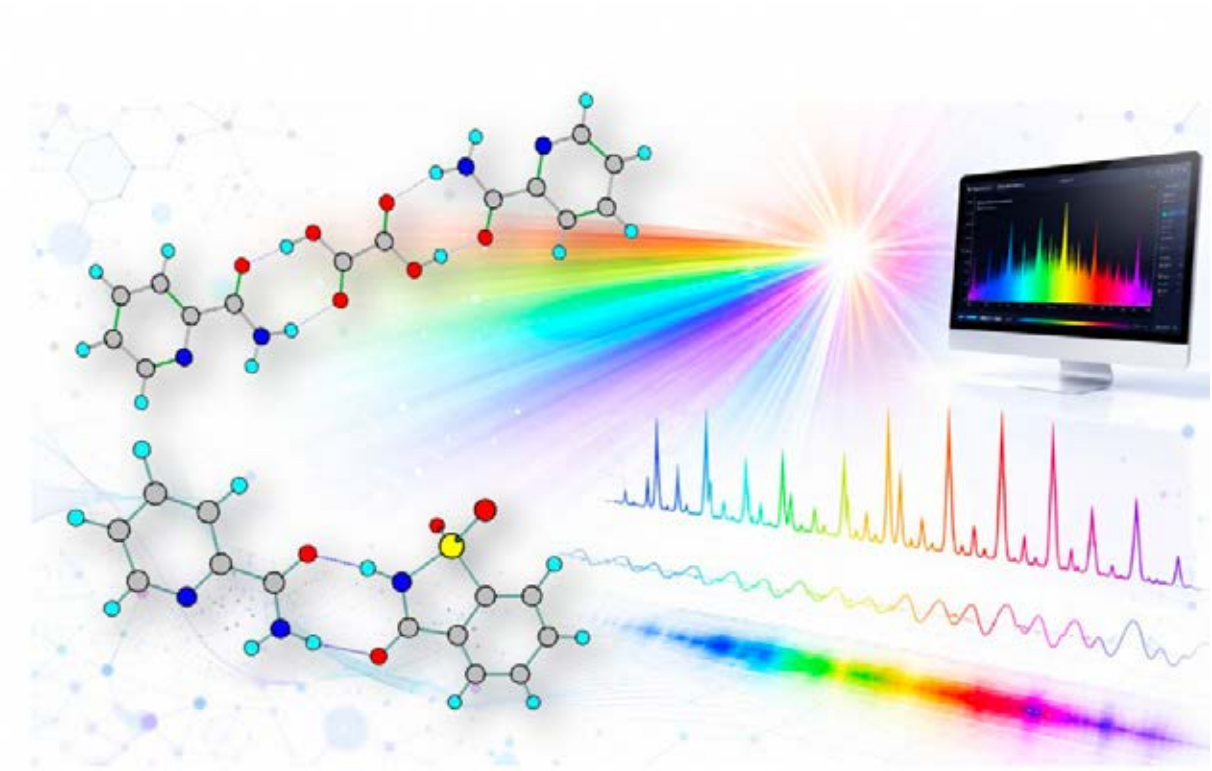
[1]*IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, Istanbul Kultur University, Ataköy Campus, Bakırköy 34156, Istanbul, Türkiye*
[2]*IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, Istanbul Kultur University, Ataköy Campus, Bakırköy 34156, Istanbul, Türkiye, Department of Physics, Faculty of Sciences and Letters, Istanbul Kultur University, Ataköy Campus, Bakırköy 34156, Istanbul, Türkiye*
[3]*IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, Istanbul Kultur University, Ataköy Campus, Bakırköy 34156, Istanbul, Türkiye, Department of Physics, Faculty of Sciences and Letters, Istanbul Kultur University, Ataköy Campus, Bakırköy 34156, Istanbul, Türkiye, CQC-IMS, Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal.*

Cocrystallization is a widely used crystal-engineering approach for the design of multicomponent crystalline materials composed of two or more neutral molecules within a single crystal lattice (Michael J. Zaworotko, J. Cryst. Growth., 1 (2007) 7). We report the design and comprehensive characterization of novel 1:1 picolinamide-saccharin (PIC-SAC) and 2:1 picolinamide-oxalic acid (PIC-OXA) cocrystals. Single-crystal X-ray diffraction confirmed the formation of new crystalline phases for both PIC-SAC and PIC-OXA. Both cocrystals crystallize in the monoclinic crystal system, and their crystal structures reveal well-defined supramolecular architectures stabilized by strong hydrogen-bonding interactions involving the amide group of picolinamide serve as the primary structure-directing force. Raman spectroscopy, together with FTIR and thermal analysis, confirmed the formation of new crystalline phases. Computational studies were further employed to correlate structural features with vibrational signatures and to characterize in detail the dominant intermolecular interactions responsible for crystal stabilization. The results demonstrate the strong influence of hydrogen-bonding motifs on both crystal architecture and vibrational behavior.

Acknowledgements: This work has been funded by the European Union, through the Horizon-Widera-2023-Talents-01 ERA-Chair 101184899 Spectroscopy@IKU "Manipulating and Characterizing Molecular Architectures: From Isolated Molecules to Molecular Crystals".

Keywords: Picolinamide, Saccharin, Oxalic acid, Cocrystal, Spectroscopy, SCXRD

Fig.1 Main structural motifs of the PIC-OXA and PIC-SAC cocrystals (artistic representation).



[Abstract:0560] [Materials]

Structural and Spectroscopic Investigation of İsoniazid-Based Cocrystal Systems

***Neris Inci Inan*[1], *Ainur Syeitkhajy*[1], *Gulce Ogruc Ildiz*[2], *Rui Fausto*[3]**

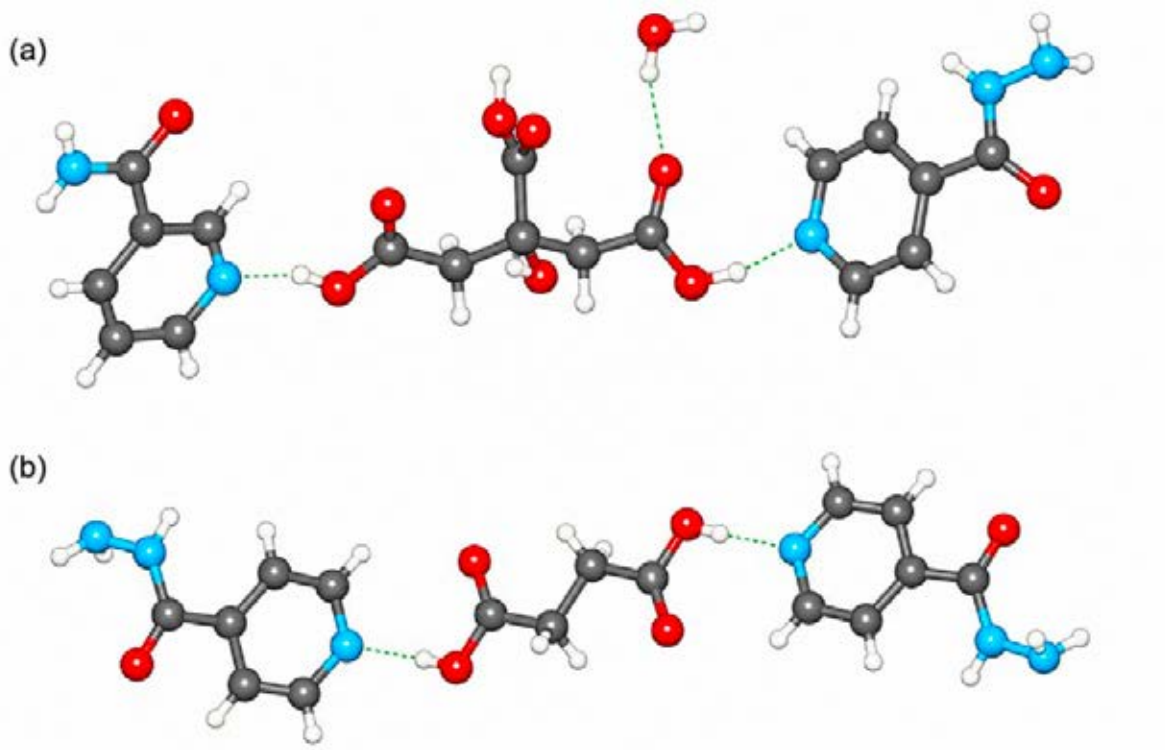
[1]*Spectroscopy@IKU, IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Turkiye*
[2]*Spectroscopy@IKU, IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Turkiye, Department of Physics, Faculty of Sciences and Letters, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Turkiye*
[3]*Spectroscopy@IKU, IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Turkiye, Department of Physics, Faculty of Sciences and Letters, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Turkiye, CQC–IMS, Department of Chemistry, University of Coimbra, 3004–535 Coimbra, Portugal*

Two isoniazid-based multicomponent crystal forms, a quaternary isoniazid-citric acid-niacinamide-water cocrystal (1:1:1:1 molar ratio) and an isoniazid-succinic acid cocrystal (2:1 molar ratio) were synthesized and investigated using a multi-technique approach. Single-crystal X-ray diffraction provided detailed crystallographic information for both solid-state forms. Both structures crystallize in the monoclinic crystal system. The quaternary cocrystal belongs to the C2/c space group, while the isoniazid-succinic acid cocrystal crystallizes in the $P2_1/n$ space group. Raman and infrared spectroscopy were used to characterize vibrationally and obtain additional information on structural aspects of the cocrystals. Band shifts and intensity changes observed in the spectra could be correlated with differences in the dominant intermolecular interactions and crystal packing of the two crystal forms. Computational studies were also performed to evaluate intermolecular interactions governing crystal packing.

Acknowledgements: This work has been funded by the European Union, through the Horizon-Widera-2023-Talents-01 ERA-Chair 101184899 Spectroscopy@IKU "Manipulating and Characterizing Molecular Architectures: From Isolated Molecules to Molecular Crystals".

Keywords: Isoniazid cocrystals, SC-XRD, Raman spectroscopy, Infrared spectroscopy, Intermolecular interactions

Fig. 1 Detail of the structural arrangement in (a) the quaternary isoniazid-citric acid-niacinamide-water cocrystal and (b) the isoniazid-succinic acid cocrystal, highlighting the main intermolecular interactions



Posters

[Abstract:0562] [Biology/Biomedicine]

AI-Assisted Surface-Enhanced Raman Spectroscopy from Spectral Fingerprints to Diagnosis

***Omer Aydin*[1], *Münevver Akdeniz*[1], *Zakarya Al-shaebi*[1], *Pınar Sağıroğlu*[2], *Mustafa Altay Atalay*[2], *Serra Ilayda Yerlitas Taştan*[3], *Gözde Ertürk Zararsız*[3], *Gokmen Zararsiz*[3], *Muzaffer Keklik*[4], *Alısan Kayabolen*[5]**

[1]*Department of Biomedical Engineering, Erciyes University, Kayseri, Türkiye*
[2]*Department of Medical Microbiology, Erciyes University, Kayseri, Türkiye*
[3]*Department of Biostatistics, Erciyes University, Kayseri, Türkiye*
[4]*Department of Hematology, Erciyes University, Kayseri, Türkiye*
[5]*Department of Medical Biology, Koc University, Istanbul, Türkiye*

Surface-enhanced Raman Spectroscopy (SERS) has attracted growing attention in medicine because of its strong potential for molecular fingerprinting, biomarker discovery, and disease diagnosis. Although substantial progress has been achieved in the physical, material, and nanostructural design of Raman-active and SERS platforms, the routine clinical implementation of these technologies remains limited. This gap is driven not only by challenges in reproducibility and spectral variability, but also by the difficulty of extracting robust and clinically meaningful information from highly complex biological datasets. Therefore, advancing Raman-based diagnostics requires not only improved sensing platforms but also application-oriented studies focused on direct analysis of real biological and clinical samples.

In this context, artificial intelligence (AI)-assisted SERS has emerged as a powerful strategy to overcome current translational barriers and move spectral technologies closer to clinical practice. By enabling advanced interpretation of large, heterogeneous, and information-rich spectral datasets, AI can improve classification performance, reduce the impact of noise and variability, and reveal subtle biochemical signatures associated with disease states. In this talk, we will present our AI-assisted SERS studies across diverse biologically and clinically relevant applications, including the detection of antimicrobial resistance-related profiles, the discrimination of cancer directly from serum samples, the classification of bacteria-associated infection signatures in serum, and the analysis of virus-like particles and extracellular vesicles. Our findings demonstrate that the integration of AI with SERS provides a robust framework for multiclass classification and clinically relevant spectral interpretation, highlighting its promise for disease diagnosis, liquid biopsy, and infection monitoring. Overall, this approach represents an important step toward transforming spectral fingerprints into actionable diagnostic insight.

This work has been partially supported by the Erciyes University Scientific Research Projects Coordination Unit (BAP) under grant number: FBAÜ-2023-12265.

Keywords: Surface-enhanced Raman spectroscopy, artificial intelligence, diagnosis, exosome, virus like particles, antimicrobial resistance

Posters

[Abstract:0566] [SERS/TERS/Plasmonics]

Machine Learning-Assisted Deep-UV SERRS for Ultra-Trace Detection and Classification of Nitroaromatic Explosives via in situ Sn-Decorated Aluminum Nanorod Arrays

Lakshay Bhardwaj, Jp Singh

Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi, 110016, India

Rapid and reliable detection of trace explosive compounds is a critical challenge in security screening, environmental surveillance, and forensic analysis. Surface-enhanced Raman spectroscopy (SERS) enables ultrasensitive molecular detection; however, its translation to the deep-ultraviolet (DUV) regime is constrained by the scarcity of scalable, chemically stable UV-plasmonic substrates. DUV excitation is inherently advantageous because the Raman scattering cross section increases with the fourth power of the excitation frequency, fluorescence backgrounds are strongly suppressed, and many biomolecules and nitroaromatic explosives exhibit intense π–π^* electronic transitions in the UV, thereby enabling resonance Raman enhancement. Aluminium is particularly attractive due to its broadband plasmonic response extending into the deep-UV and its compatibility with large-area, low-cost fabrication. Here, these limitations are addressed through a hybrid architecture consisting of Sn nanoparticle–decorated Al nanorod arrays fabricated by glancing angle deposition. The high-aspect-ratio Al nanorods provide strong electromagnetic field confinement, while Sn decoration tunes the local dielectric environment, promotes interfacial charge-transfer interactions, and mitigates oxidation-induced plasmonic losses. The resulting substrates exhibit a robust and reproducible deep-UV plasmonic response, delivering substantial SERRS enhancement for adenine and $Ru(bpy)_3^{2+}$. Furthermore, ultrasensitive detection of nitroaromatic explosives, including 2,4-dinitrotoluene (DNT), p-nitrobenzoic acid (PNBA), and picric acid, is achieved through multiplex measurements and machine-learning-assisted classification. These results establish Sn nanoparticle–decorated Al nanorod arrays as a scalable and effective deep-UV SERRS platform for security-oriented sensing applications.

Keywords: resonance Raman scattering, deep-UV Raman sensing, trace explosive detection, label-free sensing, machine learning

[Abstract:0567] [Materials]

From Co-Crystal to Amorphous Phase and Back: Matrix Isolation Spectroscopy and Computational Investigation of the Reversible Phase Transformation Pathways of the Isoniazid-Gallic Acid System

***Dilara Kaplanoğlu*[1], *Gulce Ogruc Ildiz*[1], *Rui Fausto*[2], *António Jorge Lopes Jesus*[3], *Bruna Costa*[2]**

[1]*IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center and Department of Physics, Faculty of Science and Letters, Istanbul Kultur University, Atakoy Campus, Bakirkoy, Istanbul, Türkiye*
[2]*IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center and Department of Physics, Faculty of Science and Letters, Istanbul Kultur University, Atakoy Campus, Bakirkoy, Istanbul, Türkiye, CQC-IMS, Department of Chemistry, University of Coimbra, 3004-535 Coimbra, Portugal*
[3]*CQC-IMS, Faculty of Pharmacy, University of Coimbra, 3000-548 Coimbra, Portugal*

Isoniazid (INH) is an antitubercular drug with high antibacterial efficacy against Mycobacterium tuberculosis, although its clinical use is associated with a risk of drug induced liver injury [1,2]. Gallic acid (GA), a natural phenolic compound possessing antioxidant and anti-inflammatory properties, is limited by its low oral bioavailability [3]. Co-crystal engineering offers an attractive strategy to improve the physicochemical and biopharmaceutical properties of such compounds without altering their molecular structures. In this work, a 1:1 INH-GA co-crystal was synthesized and structurally characterized using Single Crystal X-ray Diffraction (SCXRD), Raman spectroscopy, and FTIR spectroscopy. The co-crystal was subsequently investigated through cryogenic FTIR spectroscopy to elucidate its solid-state transformation pathways. Following sublimation under high vacuum, the material was deposited at 15 K either in an argon matrix or as pure material. Spectroscopic analyses revealed that the coformers were deposited as independent molecular species. Temperature dependent FTIR measurements demonstrated that heating of the deposited material or of the material resulting from Ar evaporation (in both cases a INH-GA co-amorphous phase) up to room temperature induced crystallization after a certain period of time, resulting in regeneration of the original co-crystal. To support the experimental observations, vibrational spectra calculated for several INH-GA dimers representing the principal crystal synthons were compared with the experimental spectra. The combined experimental and computational results provide detailed insight into the reversible co-crystal/amorphous phase transformations, demonstrating the usefulness of cryogenic spectroscopy for investigating phase evolution in pharmaceutical multicomponent solids.

References:

1. Q. Chai, Y. Zhang, C. H. Liu, Front. Cell. Innfect. Microbiol., 8 (2018) 158.

2. Timmins, G. S.; Deretic, V. Mol. Microbiol., 62, 2006, 1220–1227.

3. P. Chen, F. Zou, W. Liu, Front. Pharmacol., 16 (2025) 1549526.

Acknowledgements: This study has been funded by the European Union, under Horizon-Widera-2023-Talents-01 ERA-Chair 101184899 (“Spectroscopy@IKU: Manipulating and Characterizing Molecular Architectures: From Isolated Molecules to Molecular Crystals”). The research was partially conducted at the Coimbra Laser Lab. Funded by the European Union under HE-GA 101131771 Lasers4EU [access PID:41248].

Keywords: Matrix Isolation Spectroscopy, Isoniazid, Gallic Acid, Co-crystal

[Abstract:0568] [Materials]

Spectroscopic Evidence for the Formation of a New Prothionamide–Caffeine Crystalline Phase

***Merve Durmus*[1], Rezvan Mohammadi[2], Irem Sultan Yildiz[2], Göktuğ İsmail Kurtuldu[2], Berkay Ede[2], Ayberk Yilmaz[3], Nihal Sarier[4], Gulce Ogruc Ildiz[5], Rui Fausto[6]**

[1]*Spectroscopy@IKU, IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, and Department of Common Courses, Rectorate, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Türkiye.*
[2]*Spectroscopy@IKU, IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Türkiye*
[3]*Spectroscopy@IKU, IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Türkiye, and Department of Physics, Faculty of Science, Istanbul University, Vezneciler, 34134 Istanbul, Türkiye 2*
[4]*Spectroscopy@IKU, IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, and Civil Engineering Department Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Türkiye*
[5]*Spectroscopy@IKU, IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, and Department of Physics, Faculty of Sciences and Letters, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Türkiye*
[6]*Spectroscopy@IKU, IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, and Department of Physics, Faculty of Sciences and Letters Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Türkiye and IMS-CQC, Department of Chemistry, University of Coimbra, P3004-535 Coimbra, Portugal*

Prothionamide is a thioamide-based antitubercular drug whose pharmaceutical application is limited by its low aqueous solubility [Cryst. Growth Des. 2023, 23, 5770–5784]. The development of multicomponent crystalline materials has become an attractive approach for modifying the physicochemical properties of active pharmaceutical ingredients while preserving their molecular integrity [Acta Pharm. Sin. B. 2021, 11, 2537–2564]. In the present study, a new crystalline phase composed of prothionamide and caffeine was prepared and characterized by FTIR and Raman spectroscopy, differential scanning calorimetry (DSC), optical microscopy, and powder X-ray diffraction (PXRD).

Crystallization experiments performed in ethyl acetate, acetonitrile, and acetone showed that acetonitrile was the only solvent leading to the formation of the new phase. Optical microscopy revealed elongated plate-like crystals with a morphology clearly distinct from those of the individual components. Significant modifications were observed in both the FTIR and Raman spectra, particularly in the hydrogen-bond-sensitive high-wavenumber region, but also throughout the fingerprint region. These spectral changes indicate alterations in the intermolecular interactions and molecular arrangement within the crystal lattice, compared to the crystals of the neat components.

DSC measurements revealed a well-defined endothermic transition with Tm (onset) = 124.0 °C, distinctly different from the melting behavior of pure prothionamide (144.4 °C) and caffeine (235.16 °C). PXRD analysis provided additional evidence for the formation of a new crystalline phase, exhibiting diffraction features that could not be reproduced by a simple combination of the individual components. The combined spectroscopic, thermal, microscopic, and diffraction results consistently support the existence of a previously unreported prothionamide–caffeine crystalline phase and provide insight into its structural organization and intermolecular interactions.

Acknowledgements: The authors thank the Horizon-Widera-2023-Talents-01 ERA-Chair 101184899 Spectroscopy@IKU “Manipulating and Characterizing Molecular Architectures: From Isolated Molecules to Molecular Crystals”, which is Funded by the European Union. The IMS-CQC is funded by the Portuguese

Science Foundation (FCT), projects UIDB/00313/2025 (https://doi.org/10.54499/UIDB/00313/2025), UIDP/00313/ 2025 (doi.org/10.54499/UIDP/ 00313/2025) and IMS-LA/P/0056/2020 (doi.org/10. 54499/ LA/P/ 0056/ 2020).

Keywords: Prothionamide–Caffeine Crystalline Phase, Solid-state characterization, Structural and vibrational characterization

[Abstract:0569] [Novel Approaches]

Raman Endophenotyping of Fabry Disease: A Framework for Precision Biomarker Discovery

***Kubra Telli*[1], Öykü Yalavuz[2], Burçak Gül Keşan[2], Alkım İbrahim Dikerler[2], Gulce Ogruc Ildiz[3], Rui Fausto[2]**

[1]*Istanbul Kültür University, Department of Molecular Biology and Genetics, Türkiye*
[2]*Spectroscopy@IKU, IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, Istanbul Kultur University, Ataköy Campus, Bakırköy 34156, Istanbul, Türkiye*
[3]*Department of Physics, Faculty of Sciences and Letters, Istanbul Kultur University, Ataköy Campus, Bakırköy 34156, Istanbul, Türkiye*

Fabry disease (FD) is an X-linked lysosomal storage disorder caused by pathogenic variants in the GLA gene, resulting in deficient α-galactosidase A activity and progressive accumulation of globotriaosylceramide (Gb3) and globotriaosylsphingosine (lyso-Gb3) within multiple tissues and biological fluids. Although lyso-Gb3 has emerged as a clinically valuable biomarker, growing evidence suggests that Fabry disease involves broader biochemical perturbations, including membrane remodeling, altered lipid organization, protein dysregulation, and chronic cellular stress. Capturing these multidimensional molecular changes remains a significant challenge for conventional biomarker strategies. Raman spectroscopy offers a label-free, non-destructive approach for interrogating complex biochemical phenotypes via vibrational molecular signatures. Rather than focusing exclusively on individual metabolites, Raman-based analyses can characterize disease-associated endophenotypes that reflect the integrated biochemical consequences of lysosomal dysfunction. From this perspective, we propose a conceptual framework for Raman endophenotyping of Fabry disease based on spectral regions associated with lipid composition, membrane architecture, and protein structure. Candidate vibrational features include C–C skeletal stretching modes (1060–1130 cm^{-1}), lipid-associated bands near 1300 and 1445 cm^{-1}, Amide I and unsaturated lipid vibrations around 1655 cm^{-1}, and CH_2 stretching modes within the 2850–2885 cm^{-1} region. Together, these spectral domains may provide complementary information regarding glycosphingolipid accumulation and its downstream biochemical effects. We further discuss how Raman spectroscopy, combined with chemometric analysis and machine-learning approaches, could facilitate the identification of spectroscopic signatures associated with disease severity, therapeutic response, and longitudinal monitoring. Establishing robust Raman endophenotypes may expand current biomarker paradigms and support the development of precision diagnostic strategies for Fabry disease.

Keywords: Fabry disease, Raman spectroscopy, Endophenotyping, Precision biomarkers

[Abstract:0571] [Materials]

Structural Characterization and Thermal Reactivity of Isoniazid-Saccharin Species: From Salts to Adduct

***Rezvan Mohammadı*[1], *Nihal Sarier*[2], *José António Paixão*[3], *Gulce Ogruc Ildiz*[4], *Rui Fausto*[5]**

[11]Spectroscopy@IKU, IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Türkiye.
[2]2Department of Civil Engineering, Faculty of Engineering, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Türkiye.
[3]3CFisUC, Department of Physics, University of Coimbra, 3004–516 Coimbra, Portugal.
[4]4 Department of Physics, Faculty of Sciences and Letters, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Türkiye.
*[5]5CQC–IMS, Department of Chemistry, University of Coimbra, 3004–535 Coimbra, Portugal. *Corresponding Author Email: sp.rezvanm@iku.edu.tr*

This work presents a green chemistry perspective on the behavior of isoniazid (INH)-saccharin (SAC) systems, emphasizing sustainable synthesis of INH-SAC salts and their transformation into a valuable adduct product. Initially, INH-SAC salts (an anhydrous and a mono-hydrated form) were prepared using simple solvent-assisted methods, where water an environmentally benign solvent enabled controlled formation of the hydrated and anhydrous crystalline forms. A key highlight of this study is the discovery of a solvent free, solid-state pathway to form a new covalent hydrazide amide adduct. Upon heating, the salts undergo thermal transformation without the need for additional solvents, catalysts, or reagents. This reaction proceeds through nucleophilic acyl substitution, involving ring opening of saccharin ring. Such a transformation demonstrates high atom economy and minimizes byproducts, making it an efficient and sustainable approach. Spectroscopic methods (Raman and infrared) and thermal analysis provided non-destructive means to monitor the process, further reducing environmental impact. Structural and computational studies supported the understanding of intermolecular interactions. As a whole, this study presents an eco-friendly route to synthesize a complex organic adduct, highlighting the potential of green chemistry strategies in pharmaceutical and materials development.

Keywords: Saccharin, Isoniazid, Adduct, SC-XRD, Spectroscopy, Thermal analysis.

Figure1

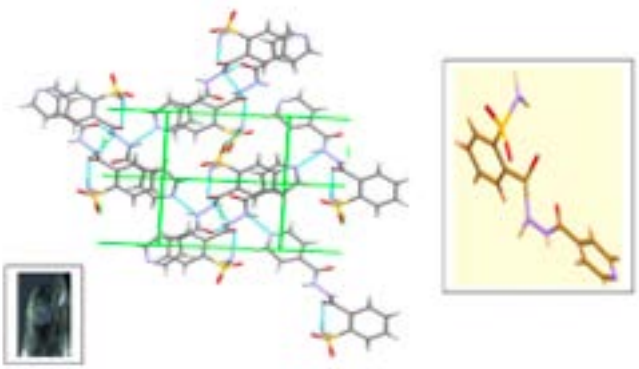


Figure 1: Single-crystal X-ray diffraction determined crystal structure of the INH-SAC adduct.

[Abstract:0572] [Novel Approaches]

Spectrikus: A Robust Computational Framework For Stochastic Deconvolution And Multi-Model Statistical Analysis of Vibrational Spectra

***Bahadır Bozkurt*[1], *Ayberk Yılmaz*[2], *Gulce Ogruc Ildiz*[3], *Rui Fausto*[4]**

[1]*Spectroscopy@IKU, IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Türkiye.*
[2]*Spectroscopy@IKU, IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Türkiye,Department of Physics, Science Faculty, Istanbul University, Vezneciler 34118, Istanbul, Türkiye*
[3]*Spectroscopy@IKU, IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Türkiye,Department of Physics, Faculty of Sciences and Letters, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Türkiye.*
[4]*Spectroscopy@IKU, IKU-SPECTRA Molecular Sciences and Spectroscopy Applied Research Center, Istanbul Kultur University, Atakoy Campus, Bakirkoy 34156, Istanbul, Türkiye,CQC-IMS, Department of Chemistry, University of Coimbra, P3004/535 Coimbra, Portugal*

Reliable deconvolution of vibrational spectral features remains a methodological challenge, particularly when multiple overlapping bands with different intrinsic profiles are considered. Multiple statistically plausible peak-fitting solutions exist, which are heavily dependent on the chosen initial conditions. Since conventional deterministic fitting workflows converge to a single local optimum, this conceals the intrinsically non-unique nature of spectral band decomposition and limits the reliability of spectral interpretation. To address this limitation, we present SPECTRIKUS, a computational framework for stochastic band deconvolution and ensemble-based evaluation of statistical models. SPECTRIKUS is a sophisticated, high-performance desktop application engineered for the automated deconvolution and rigorous statistical assessment of complex, overlapping spectral envelopes, with primary applicability to infrared and Raman spectroscopy.

SPECTRIKUS employs a multi-start nonlinear least-squares optimization strategy, generating numerous independent fits from randomized initial conditions and thus implementing a stochastic multi-start optimization paradigm. This approach facilitates an exhaustive exploration of the solution space by executing hundreds of independent nonlinear least-squares minimizations derived from randomized initial conditions. The system aggregates all solutions that surpass a user-defined coefficient of determination (R^2) threshold. To ensure the physical and statistical validity of the models, each candidate solution is scrutinized using an array of information-theoretic model-selection criteria including Akaike Information Criterion, corrected Akaike Information Criterion, Bayesian Information Criterion, and adjusted R^2 which penalize over-parameterization and mitigate the risk of spurious band proliferation.

A defining feature of the SPECTRIKUS architecture is its integrated unsupervised machine learning pipeline, designed to analyze the resulting solution ensemble. This pipeline incorporates several advanced dimensionality-reduction techniques and distinct clustering algorithms. This allows users to distinguish genuinely alternative interpretations of band structure from minor variations in fitting parameters.

The platform offers comprehensive pre-processing capabilities, including state-of-the-art baseline correction, alongside various smoothing filters and normalization modes. Methodological integrity and traceability are

maintained through a persistent undo/redo history stack. Results can be exported as structured Excel workbooks or comprehensive multi-page PDF reports.

This work was supported by the European research Agency via the European Research Agency ERA-Chair 101184899, Spectroscopy@IKU “Manipulating and Characterizing Molecular Architectures: From Isolated Molecules to Molecular Crystals”.

Keywords: Spectral profiles deconvolution, stochastic optimization, ensemble-based model selection

[Abstract:0579] [Industrial/Societal Applications]

FAIR Analytical Data for Safe and Sustainable by Design

***Nina Jeliazkova*[1], *Raquel Portela*[2], *Nikolay Kochev*[1], *Luchesar Iliev*[1], *Egon Willighagen*[1], *Sergey Soroka*[1], *Nicolás Coca López*[2], *Miguel Bañares*[2]**

[1]*Ideaconsult Ltd, Sofia, Bulgaria*
[2]*Instituto de Catalisis y Petroleoquimica (ICP), CSIC, Madrid, Spain*

Analytical data is a cornerstone of the Safe and Sustainable by Design (SSbD) framework, enabling material characterization, hazard assessment, and property modeling for emerging materials. However, analytical data generated across laboratories and techniques is often fragmented, inconsistently described, and difficult to reuse, limiting its integration into computational workflows and decision-support systems.

We present spectra.adma.ai, an open, FAIR, multi-technique analytical database designed to address these challenges through standardized data structuring and harmonization. The platform is built on the NeXus data model and implemented as an open-source system leveraging the ramanchada2 framework for Raman spectroscopy data processing, calibration, and harmonization workflows (Georgiev et al., 2025, Journal of Raman Spectroscopy, https://doi.org/10.1002/jrs.6789). This provides a reproducible infrastructure for spectroscopic data handling and consistent reference alignment across instruments and laboratories.

The database integrates curated datasets from interlaboratory studies and research projects, including Raman reference materials developed through community calibration efforts, as well as plastics and bioplastics characterization datasets. Standardized metadata structures and harmonized formats ensure interoperability and enable cross-study reuse across materials science applications.

A central feature is integration with Electronic Laboratory Notebooks (ELNs), supporting automated data capture and reducing co-creation gaps between experimental generation and data curation. This directly supports SSbD workflow digitalization as described in the ELN-based automation framework (Jeliazkova et al., 2026, GCSM Proceedings, https://doi.org/10.1007/978-3-032-21157-6_29).

Importantly, this infrastructure is aligned with emerging AI-driven approaches in spectroscopy and SSbD. Recent work demonstrates that combining open science principles, FAIR data infrastructures, and machine learning enables robust AI-powered Raman spectroscopy workflows and improved spectral interpretation capabilities (Coca-Lopez et al., 2025, ACS Nano, https://doi.org/10.1021/acsnano.5c09165). In this context, the platform is designed as an enabling layer for AI-ready analytical ecosystems, supporting machine learning applications for spectral analysis, property prediction, and uncertainty-aware hazard assessment within SSbD workflows.

Keywords: Safe and Sustainable by Design (SSbD), FAIR data management, Multi-technique spectroscopy databases, NeXus data format Automated workflows, Electronic laboratory notebooks (ELN) integration

Posters

[Abstract:0582] [Novel Approaches]

A Simple and Fast Portable Raman Method for the Identification of Illegal Adulterants in CLA Dietary Supplements through Chemometrics

***Sukriye Nihan Karuk Elmas*[1], *Beyza Eksim*[1], *Muhammad Tariq Shah*[2], *Fatma Nur Arslan*[3], *Muhammed Yunus Bektay*[4], *Demet Akalgan Aklar*[5]**

[1]*Department of Analytical Chemistry, Faculty of Pharmacy, Istanbul University–Cerrahpaşa, Istanbul, Turkiye*
[2]*Higher Education Department, Khyber Pakhtunkhwa, Government Degree College Tangi, Charsadda, Pakistan*
[3]*Department of Chemistry, K.O. Faculty of Science, University of Karamanoglu Mehmetbey, Karaman, Turkiye*
[4]*Department of Clinical Pharmacy, Faculty of Pharmacy, Istanbul University–Cerrahpaşa, Istanbul, Turkiye*
[5]*Department of Pharmacy Management, Faculty of Pharmacy, Istanbul University–Cerrahpaşa, Istanbul, Turkiye*

In this study, simple fast Raman spectroscopy methods were proposed for the identification of adulterants in conjugated linoleic acid (CLA) dietary supplements through chemometrics. The effortless methods were developed by using compact Raman spectrometer allied with soft independent modeling of class analogy (SIMCA) and partial least squares–regression (PLS–R) analyses. The models of SIMCA and PLS–R were constructed to assess quantitative detection limits for different illegal adulterants (sibutramine, phenolphthalein, 1,3-dimethylamylamine, yohimbine and dinitrophenol) in commercial CLA supplements. The methods were successful in the quantitative identification of these adulterants in the supplements bought from pharmacy; they could detect the illegal targets at realistic adulteration levels (0–10%; w/w), confirming the potential of compact Raman spectroscopy based methodologies for quick screening applications. Thus, compact Raman spectroscopy combined with chemometrics is expected to become an increasingly powerful and reliable analytical tool for the detection of adulteration and fraud in dietary supplements in the coming years.

Keywords: Raman, Adulteranteration, CLA, Supplement, Chemometrics

[Abstract:0584] [Materials]

Optical-Photothermal Infrared (O-PTIR) Microspectroscopy for Simultaneous Submicron Infrared and Raman Analysis of Calcified Materials

***Carolin Borbeck*[1], *Miriam Unger*[1], *Mustafa Kansiz*[2]**

[1]*Photothermal Spectroscopy Corp GmbH, Landgrafenstr. 12, 45476 Mülheim an der Ruhr, Germany*
[2]*Photothermal Spectroscopy Corp, 325 Chapala Street, Santa Barbara, CA 93101, USA*

Calcifications serve vital roles in both health and disease, acting as biomarkers for breast cancer and as structural components in bone and teeth. Traditional analytical methods, such as Fourier Transform Infrared (FTIR) and Raman spectroscopy, are often constrained by limitations in spatial resolution, sensitivity to water interference, or the need for complex sample preparation. Optical Photothermal Infrared (O-PTIR) spectroscopy overcomes these limitations by enabling label-free, contact-free chemical imaging with unprecedented submicron spatial resolution.

O-PTIR combines photothermal excitation using a tunable infrared laser and detection through visible light scattering, enabling infrared absorption spectra to be obtained with high spatial precision. Simultaneous Raman spectra are captured using the same optical path, allowing complementary molecular information to be acquired at the same submicron resolution without sample contact. Samples of breast cancer calcifications, bone, and teeth were analyzed to assess mineral content, matrix composition, and heterogeneity.

The technique successfully mapped carbonate and phosphate content variations in breast cancer microcalcifications, revealing compositional heterogeneity correlated with pathological states. In bone and dental samples, O-PTIR provided detailed insight into mineral phase distribution, protein matrix organization, and hydration status. The simultaneous collection of Raman spectra enriched the analysis by highlighting molecular features not captured by infrared alone.

In conclusion, O-PTIR spectroscopy represents a paradigm shift in the molecular imaging of calcified materials. Its ability to perform non-contact, simultaneous submicron infrared and Raman analysis with high chemical specificity positions it as a powerful tool for advancing biomedical research, diagnostics, and biomaterials development.

Keywords: O-PTIR, Multimodal Spectroscopy, Vibrational Microscopy, Calcified Biological Material

[Abstract:0587] [Biology/Biomedicine]

Rapid phenotypic drug susceptibility testing of *Mycobacterium tuberculosis* by single-cell Raman spectroscopy with deuterium isotope probing

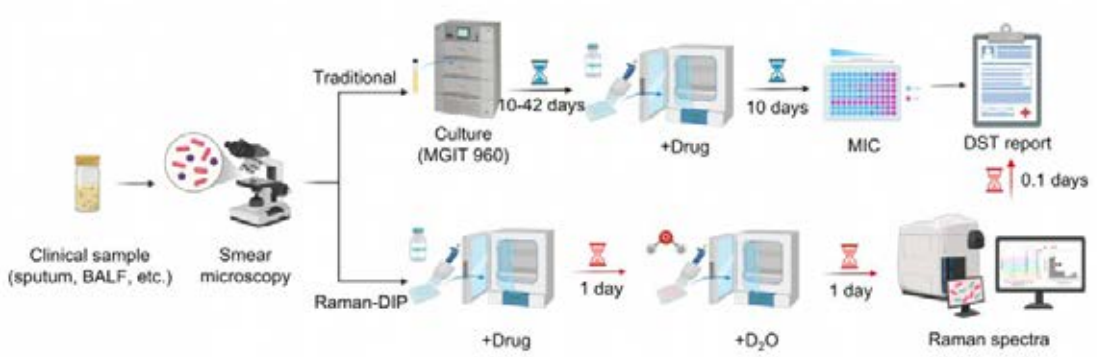
***Xin Mao*[1], *Yiyan Song*[3], *Jingkai Wang*[4], *Dawei Yu*[3], *Huijie Hu*[1], *Ping Xu*[3], *Yiwen Cao*[2], *Zhiqiang Zhang*[1], *Junchi Xu*[3], *Wei E. Huang*[4], *Yizhi Song*[2]**

[1]*School of Biomedical Engineering (Suzhou), Division of Life Science and Medicine, University of Science and Technology of China, Suzhou 215163, China*
[2]*Suzhou Institute of Biomedical Engineering and Technology, Chinese Academy of Science, Suzhou 215163, China*
[3]*Department of Clinical Laboratory, The Fifth People's Hospital of Suzhou, The Affiliated Infectious Diseases Hospital of Soochow University, Suzhou 215163, China*
[4]*Department of Engineering Science, University of Oxford, Oxford, OX1 3PJ, United Kingdom*

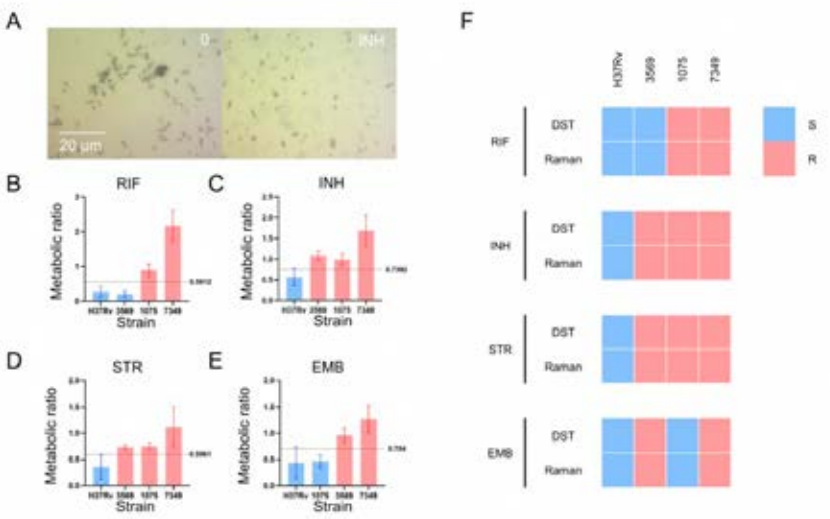
Accurate and timely drug susceptibility testing (DST) is essential for tuberculosis (TB) management, particularly in the context of rising multidrug-resistant *Mycobacterium tuberculosis* (MTB). However, conventional culture-based methods are slow, and molecular assays cannot fully account for resistance beyond known mutations. Here, we present a rapid phenotypic DST (pDST) workflow for MTB based on single-cell Raman spectroscopy combined with deuterium isotope probing (Raman-DIP). Following optimization of antibiotic exposure and D_2O labeling conditions for MTB, the workflow enabled phenotypic readout within approximately 50 h. Using five MTB strains and four first-line anti-tuberculosis drugs, Raman-DIP clearly distinguished drug-sensitive from drug-resistant strains and showed 100% categorical agreement with the reference broth-based method in the tested strain set. In simulated sputum samples, the method also achieved 100% classification accuracy, supporting its feasibility in a sputum-like matrix. In pure cultures, Raman-DIP further enabled quantitative minimum inhibitory concentration (MIC) determination, with MIC estimates consistent with reference values for the examined strain-drug combinations. These results support Raman-DIP as a rapid and biosafe phenotypic platform for MTB drug susceptibility testing, with potential value for earlier and more individualized therapeutic decision-making.

Keywords: Mycobacterium tuberculosis (MTB), single-cell Raman spectroscopy, deuterium isotope probing, phenotypic drug susceptibility testing (pDST)

Workflow comparison between conventional and Raman-DIP pDST for MTB.

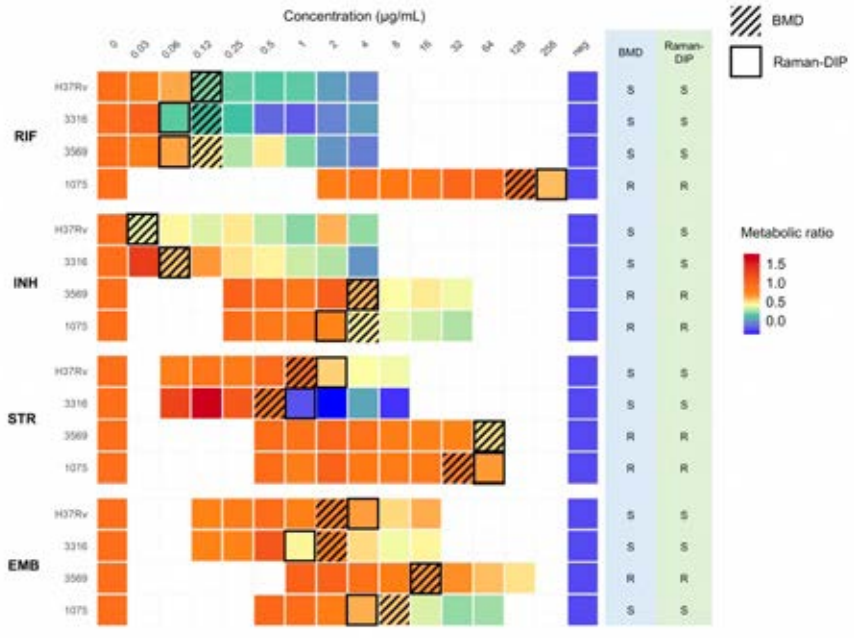


Raman-DIP enables pDST in simulated sputum samples.



(A) Bright-field images of simulated sputum samples spiked with MTB strain 1075 before (0 μg/mL) and after treatment with isoniazid (INH, 0.25 μg/mL). (B–E) MR of four MTB strains (H37Rv, 3569, 1075, 7349) in sputum samples treated with four first-line anti-TB drugs: (B) RIF, (C) INH, (D) STR, and (E) EMB. Dashed lines indicate the MR classification thresholds established in pure cultures. (F) Comparison of drug susceptibility results obtained by conventional broth-based pDST and Raman-DIP for each strain-drug pair. For each condition, the simulated sputum sample was derived from one processed preparation.

Heatmap visualization of MR values across four MTB strains exposed to gradient concentrations of first-line anti-TB drugs.



Each heatmap cell represents the MR of a given strain at a specific drug concentration, obtained from one culture preparation.

Posters

[Abstract:0589] [SERS/TERS/Plasmonics]

Probing the Competing Vibrational Stark Effect and Interfacial Electronic Effects in the Tunnel Junction Using Tip-Enhanced Raman Spectroscopy

***Ruonan Wang*[1], *Luyao Zhu*[2], *Yao Zhang*[2], *Jing-Juan Xu*[1], *Li-Qing Zheng*[1]**

[1]*School of Chemistry, Nanjing University, Nanjing, China*
[2]*Hefei National Research Center for Physical Sciences at the Microscale and CAS Center for Excellence in Quantum Information and Quantum Physics, University of Science and Technology of China, Hefei, China*

Vibrational frequency shifts under applied bias in molecular junctions are frequently interpreted through the vibrational Stark effect; however, interfacial electronic coupling and bias-driven molecular reorientation represent alternative, often-overlooked mechanisms. Here, we used scanning tunneling microscopy-based tip-enhanced Raman spectroscopy (STM-TERS) to investigate the bias-dependent behavior of 4-mercaptobenzonitrile (4-MBN) bound either to an Au substrate or to an Ag tip.

At sample biases from +0.2 to +2.0 V, substrate-bound 4-MBN exhibits a reversible, monotonic C≡N redshift. Concurrent changes in the relative spectral contributions of the C≡N and C–S bands are consistent with progressive molecular tilting toward the substrate. In contrast, tip-bound 4-MBN displays an initial C≡N blueshift at low bias, followed by a redshift at higher bias. Control measurements using Au tips reproduced the same nonmonotonic bias dependence, indicating that the contrasting behavior is not simply attributable to differences between the Au and Ag electrodes.

DFT calculations were performed to elucidate the spectral changes. Simulation results reveal that the vibrational Stark effect induces the blueshift of C≡N, opposite to the redshift observed for substrate-bound 4-MBN. This discrepancy indicates that the experimental redshift cannot be explained by the Stark effect alone. By contrast, further calculations incorporating metal–molecule electronic interactions show field-induced C≡N bond elongation, increased antibonding-orbital population, and enhanced interfacial charge redistribution, supporting a key role for interfacial electronic effects in the redshift of C≡N, in full agreement with the experimental results. In the Ag_{20} tip-cluster model, low-bias C≡N bond shortening is consistent with a Stark-dominated blueshift, whereas enhanced interfacial charge redistribution at higher bias is accompanied by increased antibonding-orbital population and bond elongation, providing a mechanistic explanation for the subsequent redshift.

These results demonstrate that bias-induced vibrational shifts are neither universally unidirectional nor necessarily linear, but depend on the local interfacial environment. In these STM-TERS junctions, substrate- and tip-anchored geometries modulate the balance between vibrational Stark and interfacial electronic effects. The nitrile vibration therefore serves not as a simple electric-field reporter but as a joint probe of the junction's electrostatic, structural, and electronic environment.

Keywords: STM-TERS, Vibrational Stark Effect, Interfacial Charge Redistribution, Molecular Junction, Nitrile Probe

Gold Sponsors

RENISHAW

PHOTOTHERMAL SPECTROSCOPY CORP

Silver Sponsors

HORIBA

Lightnovo

OXFORD INSTRUMENTS

Bronze Sponsors

A·P·E

attocube WITTENSTEIN group

Coblentz SOCIETY

EDINBURGH INSTRUMENTS

LIGHT CONVERSION

Refined Diagnostics

STUTTGART INSTRUMENTS INFRARED LASERS

We ♥ Spectroscopy S.T.JAPAN europe gmbh

timegate

Wasatch Photonics

Other Sponsors

Coblentz SOCIETY

StellarNet Inc

Nano Biophotonics App

XXIX ICORS

29th International Conference on Raman Spectroscopy

icors2026.org

Istanbul TÜRKİYE 23-27 August 2026