BOOK OF ABSTRACTS

SEPTEMBER 14-18 — OLOMOUC, CZECH REPUBLIC

CZECH–SLOVAK SPECTROSCOPIC CONFERENCE

September 14-18, 2026

msms

Mössbauer Spectroscopy in Materials Science 2026

Ioannes Marcus Marci Spectroscopic Society

Faculty of Science

Palacký University Olomouc

SMALT

JSVTS

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ABOUT THE CONFERENCE

The **19th Czech - Slovak Spectroscopic Conference (19th CSSC)** is a scientific meeting with international participation to share recent developments, exchange ideas, explore new directions and initiate a possible collaboration in the analytical spectrometry area. Leading scientists and researchers will be invited to present their most up-to-date results at this conference, to exchange exciting ideas and experiences, and to explore future development. The aim of this scientific event is to bring together experts from universities, academia, official centres, various laboratories, and industry, to summarize the current progress in various areas of spectroscopy/spectrometry and the trends in the applications such as chemical, environmental, geological, biological, food, pharmaceutical and industrial materials and to stimulate contacts and mutual exchange of experiences and ideas.

A series of specialised colloquia entitled **Mössbauer Spectroscopy in Material Science (MSMS)** was initiated in Central Europe. They have been regularly organised since 1994, alternatively in Slovakia and the Czech Republic, with a two-year periodicity. Firstly, MSMS colloquium represents an important forum for researchers in materials science who share their results on understanding the solid-state matter employing Mössbauer spectroscopy. Secondly, the conference organisers invite several scientists well distinguished in Mössbauer spectroscopy worldwide to give both tutorial lectures and lectures of broad perspective to convey the knowledge to young generation (researcher beginners, PhD students, etc.). Thirdly, cutting-edge works are presented, stimulating future studies and research orientation in the field of Mössbauer spectroscopy.

The microsymposium entitled **Advances in vibrational spectroscopy - Celebrating 60 years of Raman spectroscopy** in our country and dedicated to the memory of Bohuslav Strauch is the inherent part of the Conference program as a parallel session. Invited as well as short lectures within this Microsymposium will cover a wide range of topics targeted on the current advances in Raman and infrared spectroscopy and their applications. In the focus of interest will be time-resolved IR and Raman spectroscopy as well as special methods of Raman spectroscopy, namely resonance Raman scattering (RRS), and surface-enhanced /resonance/ Raman scattering (SERS and SERRS). Additionally, the development and applications of advanced techniques of vibrational spectroscopic imaging and mapping both on the micro- and the nano-scale will be covered. Furthermore, applications of IR and Raman spectroscopy in chemistry, material science, geology, gemmology, art conservation, environmental science, food processing, biology and medicine will be an inherent part of the Microsymposium scope.

CSSC & MSMS COMMITTEES

SCIENTIFIC COMMITTEE

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Tomáš Vaculovič	Masaryk University, Brno, Czech Republic
Tomáš Vašina	Ioannes Marcus Marci Spectroscopic Society, Czech Republic

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MEET THE MEDALISTS

IOANNES MARCUS MARCI MEDAL

Prof. Blanka Vlčková

Professor Blanka Vlčková graduated from the Department of Inorganic Chemistry at Charles University, Prague in 1984. Her scientific carrier progressed at the Department of Physical and Macromolecular Chemistry, Charles University where she became a full professor in 2008 and has been a professor emeritus since 2025. In 1989, she established her research group "Surface-enhanced Raman scattering" (SERS), which was the first research group in the Czech Republic which dealt with this phenomenon. Prof. Vlčková and her research group have substantially contributed to elucidation of the molecular resonance damping in surface-enhanced resonance Raman scattering(SERRS), to identification of the reduced Ag(0) adsorption on Ag nanoparticle surfaces and specification of the conditions of their formation as well as to explanation of the simultaneous operation of graphene-enhanced Raman scattering (GERS) and SERS. Since 2017, Prof. Vlčková research interests involve also the plasmon-catalysed reactions on plasmonic metal nanoparticle surfaces and establishing of their mechanisms on the basis of targeted experiments using SERS spectral detection and monitoring of the reaction progress. Prof. Blanka Vlčková published over 80 papers and two book chapters, and she delivered about 50 invited lectures at international conferences and universities abroad. She acted as the visiting scientist at University of London, University of Amsterdam, University of Toronto and University of California at Santa Barbara, and as the visiting professor at Mc. Gill University Montreal. In 2011, she was awarded "Certificate of Appreciation for Peer Review Activities" by American Chemical Society.
During her scientific carrier, Prof. Vlčková has been actively involved in the Ioannes Marcus Marci Spectroscopic Society (IMMSS) as a leader of the Vibrational Spectroscopy group and/or a head of the Molecular Spectroscopy Section. She participated in organizing and program committees of international as well as local conferences and lectured at the Vibrational Spectroscopy courses organized by the IMMSS.

Prof. Viktor Kanický

Viktor Kanický (17 June 1953) graduated in chemistry from the Faculty of Science of Jan Evangelista Purkyně University in Brno (now Masaryk University) in 1977. In 1978, he obtained the RNDr. (Rerum Naturalium Doctor) degree in Analytical Chemistry for his thesis on ternary complex-forming equilibria and the spectrophotometric determination of uranium. In 1990, he earned the CSc. degree (equivalent to Ph.D.) at the Faculty of Science, Masaryk University, for his work on the spectroscopic study of rare earth elements using inductively coupled plasma optical emission spectrometry and their determination in ores and products of technological purification processes. He habilitated in 1996 at the Faculty of Science, Masaryk University, and in 2003 was appointed Professor of Analytical Chemistry. In 2001, he was awarded the DrSc. (Doctor of Science) degree at the University of Pardubice. Following his graduation and a one-year study stay at the Faculty of Science, he worked at the Geological Survey in Ostrava (1978–1991), where he contributed to pioneering developments in inductively coupled plasma optical emission spectrometry. He subsequently joined the Faculty of Education of Masaryk University and, since 1994, has been affiliated with the Faculty of Science. He has served as principal investigator or co-investigator of numerous projects funded by the Czech Science Foundation and the Ministry of Education. From 2005 to 2007, he was Head of the Department of Analytical Chemistry, and until 2023 he served as Deputy Head of the Department of Chemistry.

Between 1999 and 2001, he was Vice-Dean for organizational affairs, editorial activities, and student social matters at the Faculty of Science. From 2010 to 2018, he served as Vice-Dean for research, doctoral studies, and international relations. From 2007 to 2010, he chaired the Doctoral Programme Board in Chemistry, and since 2019 he has chaired the Doctoral Programme Board in Analytical Geochemistry.He is also a member of doctoral programme boards in Analytical Chemistry at Masaryk University and at other institutions, including Palacký University, Jan Evangelista Purkyně University, and University of Chemistry and Technology Prague. He has served as a member of the Slovak national committee for the defence of DrSc. theses in analytical, environmental, and nuclear chemistry. He is currently a member and Vice-Chair of the Committee for awarding the Doctor of Science (DSc.) degree in Analytical Chemistry.

From 2005 to 2023, he served as the elected Chairman of the Ioannes Marcus Marci Spectroscopic Society, and since 2023 he has held the position of First Vice-Chairman. His research and teaching activities focus on optical and mass spectrometry with inductively coupled plasma, the analysis of geological samples, elemental mapping/imaging, and laser ablation combined with plasma spectrometry. He is the author or co-author of more than 170 original research articles indexed in the Web of Science, with over 3,000 citations and an h-index of 29.

In 1994, he introduced a new research direction at Masaryk University based on the analytical use of pulsed laser ablation (LA-ICP-OES, LA-ICP-MS), secured funding for instrumentation, and established a research group in this field. Together with Professor Vítězslav Otruba, he co-founded the Laboratory of Plasma Sources for Chemical Analysis in 1997, later renamed the Laboratory of Atomic Spectrochemistry, which he subsequently led. He played a key role in building instrumentation and research programmes within several Ministry of Education research plans, the CEITEC project, and the project "Research Infrastructure for Doctoral Studies in Chemistry," which he initiated and led. He also contributed to the project "Long-term Research of Geochemical Barriers for Nuclear Waste Disposal." From 2019 to 2023, he was a member of Panel 206 (Analytical Chemistry) of the Czech Science Foundation, serving first as Vice-Chair and subsequently as Chair.

In 2016, he was awarded honorary membership of the Slovak Spectroscopic Society. In 2017, he received the Tibor Török Medal from the Hungarian Spectrochemical Society of the Hungarian Chemical Society for his contributions to analytical spectroscopy. In 2024, he was awarded the Nicolaus Konkoly-Thege Medal of the Slovak Spectroscopic Society for his outstanding achievements in analytical spectroscopy.

HONORARY MEMBER OF IMMSS

Prof. Yukihiro Ozaki

Professor Yukihiro Ozaki obtained his PhD in Physical and Inorganic Chemistry at Osaka University, Japan, and he became a Professor of Chemistry at School of Science and Technology, Kwansei-Gakuin University, Japan in 1993. In 2006, he was appointed Dean of the School of Science, and in 2013 the Vice-president of Kwansei-Gakuin University.

Prof. Ozaki is the recipient of numerous international and domestic awards, e.g. Dasari Lecture Award (2011), George R. Harrison Spectroscopy Laboratory, MIT; Memorial Award for the 90th Anniversary of the Discovery of Raman Effect (2018), Bangalore, India; The Medal with Purple Ribbon from Japanese Emperor (2018) Pittsburg Spectroscopy Award, Pittsburg Spectroscopy Society, USA (2019); Charles Mann Award of Applied Raman Spectroscopy, FACSS, USA (2020), Karl Norris Award, International Council of Near-infrared Spectroscopy (2021), Ioannes Marcus Marci medal, JMM Spectroscopic Society, Czech Republic (2022) and Ellis R. Lippincot Award, Optical Society of America, USA (2025). He has presented more than 140 invited and plenary lectures at international conferences all over the world. He was a Steering Committee Member of International Conference on Raman Spectroscopy (ICORS) (2012-2018) and of International Conference on Advanced Vibrational Spectroscopy (ICAVS) (2013-2019).

Prof. Ozaki was also the Vice President of Japan Society for Analytical Chemistry (2011-2012), the President of Spectroscopical Society of Japan (2014-2016) and the Representative of Japan in Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) (2012-2017). He was also a Member of Editorial Board of spectroscopy journals, e.g. the Journal of Raman Spectroscopy and the Journal of Near-IR Spectroscopy, and an Associate Editor of Encyclopedia of Analytical Chemistry.
Prof. Ozaki published more than 1,100 papers as well as 19 books and 70 book chapters and review articles (with over 48,000 citations and h-index of 94) devoted to medical applications of Raman spectroscopy, to surface-enhanced Raman (SERS) and tip-enhanced Raman (TERS) spectroscopy, and to far-ultraviolet (FUV) and near infrared spectroscopy. In particular, Prof. Ozaki became a path breaking scientist in medical Raman spectroscopy owing to the first successful application of Raman spectroscopy to an investigation of the disease mechanism. Furthermore, he has opened a new era in FUV spectroscopy of condensed matter by introducing the attenuated total reflection (ATR) technique to the FUV region, and he has also substantially contributed to elucidation of both the electromagnetic and the chemical mechanism of SERS.

NICOLAUS KONKOLY-THEGE MEDAL

Prof. Marcel Miglierini

Marcel Miglierini graduated from the Slovak University of Technology in Bratislava in 1981, where he has been working at the Institute of Nuclear and Physical Engineering since then. In 1995, he received his DrSc. and in 1997 he was appointed full professor of condensed matter physics at the Slovak University of Technology in Bratislava. At the beginning of his scientific career, he completed several long-term research stays in Japan, France, Austria and Germany. His main areas of scientific interest include magnetic and structural properties of disordered materials (amorphous metallic glasses, quasicrystals, nanocrystals, powder steels) and their hyperfine interactions, structural positions of iron in archaeological, biological, chemical, geological, mineralogical and metallurgical systems. They were investigated mainly by nuclear spectroscopy methods (Mössbauer spectroscopy, NMR, electron-positron annihilation, gamma spectroscopy), atomic and magnetic microscopy and special analytical techniques based on synchrotron radiation. For his achievements, the Mössbauer Effect Data Center in Asheville, USA, declared him one of the four most productive authors in the field of Mössbauer spectrometry in the world in the years 1990–2000. He received awards from several institutions, including the Slovak University of Technology in Bratislava, the Slovak Physical Society, the Association of Slovak Scientific and Technical Societies and the Ioannes Marcus Marci Spectroscopic Society (IMMSS).
In 2011, prof. Miglierini initiated the Winter School of Synchrotron Radiation with international participation, where renowned experts in the field share their knowledge and skills with the participants of the school. Currently, this activity continues as the XFEL, Synchrotron and Neutron Radiation Users School. Since 1994, prof. Miglierini has organized a series of international conferences entitled Mössbauer Spectrometry in Materials Sciences, which have been held regularly every two years until now. The conferences take place alternately in Slovakia and the Czech Republic. In 2002, this event was held as the Czech-Slovak NATO Workshops for Advanced Research under the joint leadership of prof. Miroslav Mašláň from Olomouc and prof. Marcel Miglierini.
Professor Miglierini has been actively involved in several international and domestic organizations. From 1998 to 2020, he represented Slovakia in the International Board for the Application of the Mössbauer Effect as an elected member. In the CENTRALSYNC consortium, which provides access to the synchrotron source in Grenoble for researchers from the Czech Republic, Hungary and Slovakia, he represented Slovakia in 2008–2018 and served as chairman of its steering committee several times. From 2003 to 2025, he was the president of the Slovak Spectroscopic Society.

Prof. Miroslav Mašláň

Miroslav Mašláň (6 May 1957) graduated in nuclear physics from the Faculty of Physics of Belarus State University in Minsk in 1982. In 1986, he earned the CSc. degree (equivalent to Ph.D.) at the Institute of Applied Physics of Belarus Academy of Science (Minsk), for his work on „Non-destructive control method of surfaces by conversion electron Mössbauer spectroscopy". He spent his entire subsequent professional life at Palacký University in Olomouc. He habilitated in 1994 at the Faculty of Science, Palacký University, and in 2002 was appointed Professor of Applied Physics. He has served as principal investigator or co-investigator of numerous projects funded by the Czech Science Foundation, Technology Agency of the Czech Republic, Ministry of Education, Youth and Sports, and the Ministry of Industry and Trade of the Czech Republic. From 2005 to 2010, he was Head of Regional Centre of Advanced Technologies and Materials, and from 2007 to 2010 he served as Head of the Department of Experimental Physics. Between 2000 and 2006 and 2014 and 2018, he served as Vice-Rector of Palacký University, during which time, amongst other things, he initiated the establishment of the university's Science and Technology Park. From 2010 to 2014, he held the post of Rector of Palacký University.

In 1992, he introduced a new research direction at Palacky University based on nuclear resonance fluorescence (Mössbauer effect). His research and teaching activities focus on Mössbauer spectroscopy and its applications in material science, mineralogy and chemistry, methodology of Mössbauer measurements, design of spectrometers in the field of X-rays and gamma rays. For many years, he lectured students on atomic and nuclear physics. He is the author or co-author of more than 130 original research articles indexed in the Web of Science, with over 2,300 citations and an h-index of 22. Under his supervision, 19 students successfully defended their doctoral theses. He supervised more than 40 master's and bachelor's theses.

PROGRAMME

Monday 14.9.	Registration desk
16:00 – 19:00	Registration
18:00 – 22:00	Welcome drink

	Tuesday 15.9.		Room 2.001
Chair: Milde	8:30 – 9:00		Opening
	9:00 – 9:50	**Kanický**	**The Early Development of ICP Optical Spectrometry in Czechoslovakia: From the First Instruments to Modern Plasma spectrometry**
	9:50 – 10:20	Holá	LA-ICP-MS for Strategic Raw Materials: From Laser-Sample Interactions to Trace Element Analysis, Imaging and New Glass Calibration Materials
	10:20 – 10:40	Pragolab	
	10:40 – 11:00	Coffee break	
Chair: Machala	11:00 – 11.30	Dubiel	Impact of Magnetism on Lattice Vibrations
	11:30 – 11:50	Georgiadis	Carbon-Encapsulated Fe_3C Nanoparticles Formed During CVD on AISi 1095 High-Carbon Steel
	11:50 – 12:10	Andrýsková	Nanostructured Cobalt Ferrite Thin Layers Preapred by Thermally Induced Decomposition of Oxalates
	12:10 – 12:30	Kudor	^{57}Fe and ^{151}Eu Mössbauer and XRD Study of Eu-Doped Goethite Nano-Composites Prepared from Different Eu-Compound Precurzors
	12:30 – 13:00	Wang	Operando Mössbauer Spectroscopy for Single-Atom Electrocatalysts
	13:00 – 13:30	Gracheva	Mössbauer and Complementary Spectroscopic Studies of Iron in Fertilizers and Plant Tissues
	13:30 – 14:45	Lunch	
Chair: Pluháček	14:45 – 15:15	Kůsová	Optical Spectroscopy and Properties of Silicon Quantum Dots
	15:15 – 15:35	Černá	Layer-by-Layer Defect Analysis of He-Ion-Irradiated MoS_2
	15:35 – 15:55	Kubala	Mean Fluorescence Lifetime
	15:55 – 16:15	Papoušková	Extending Ambient Mass Spectrometry Using Deep-UV Laser-Based Ionization Approach
	16:15 – 16:35	Knytlová	Rapid Screening of Small Molecules Using Ambient Mass Spectrometry
	16:35 – 16:55	Palounek	Concurrent Characterization of Plasmonic Hot Spot, Molecular Structure and Molecular Mass
	17:45 – 18:00	Group photo	
	18:00 – 19:30	Poster session	

	Tuesday 15.9.		Room 2.005
	10:40 – 11:00	Coffee break	
Chair: Ozaki	11:00 – 11.30	Frank	Novel Physicochemical Phenomena in Graphene Revealed by Microdroplet In-situ Raman Spectroelectrochemistry
	11:30 – 12:00	Kalbáč	UHV Exfoliation and Spectroscopy of 2D Materials
	12:00 – 12:30	Kalbáčová Vejpravová	New Frontiers in Raman Spectroscopy of 2D Materials: Isotope Engineering and Twisted Light
	12:30 – 13:00	Profant	Towards Robust Quantitative Raman Spectroscopy: From FIngerprints to Thermodynamics
	13:00 – 13:30	Němec	Molecular Materials for Nonlinear Optics: An Integrated Approach to Phase Characterisation
	13:30 – 14:45	Lunch	
Chair: Marques	14:45 – 15:15	Žůrková	FT-IR Spectroscopy for The Non-Invasive Analysis of Paintings
	15:15 – 15:45	Mojzeš	Raman Microscopy of Crystalline Inclusions in Microalgae
	15:45 – 16:15	Kapitán	Experimental Development of Raman Optical Activity in Olomouc – Celebrating 30 Years of ROA in Our Country
	16:15 – 16:45	Kaminsky	Advanced Vibrational Spectroscopy for Chiral Solid-State Pharmaceuticals
	16:45 – 17:15	Tabor	From Molecular Vibrations to Catalytic Function: FTIR Spectroscopy in Action
	17:15 – 17:45	Matějka	Nanoscale Imaging and Nano-FTIR Spectroscopy of Surface Nano-Thin Polydopamine Films – What Is The Role of Deposition Time and Substrate Material?
	17:45 – 18:00	Group photo	
	18:00 – 19:30	Poster session	

Wednesday 16.9.		Room 2.001
Chair: Matějka		
8:30 – 9:20	**Vlčková**	**The Role of Surface-Adsorbate Bonding in SERRS and in Plasmon Catalysis**
9:20 – 9:50	Schlücker	SERS-Based Biophotonics: From Nanotags to Lateral Flow Assays 2.0
9:50 – 10:10	Klimiček	Modern Approach to Raman Microscopy – RAMANTouch
10:10 – 10:30	Coffee break	
Chair: Schünemann		
10:30 – 11:00	Szumiata	Mössbauer Spectroscopy and Magnetic Methods for Environmental Monitoring in Industrial and Post-Industrial Areas
11:00 – 11:30	Kubuki	^{57}Fe-Mössbauer Study of Photo-Fenton Catalyst Prepared from Domestic Waste Slag
11:30 – 11:50	Machala	Molybdenum-Modified Iron Oxides as Catalysts for Degradation of Meropenem by Peroxydisulfate
11:50 – 12:10	Kalusová	Spectroscopic and Photocatalytic Study of β-Fe_2O_3 Prepared in The Presence of Alkali Chlorides
12:10 – 12:30	Dubiel	Lattice Dynamics and Magnetism of Two Sigma-Phase FeCrNi Compounds: Mössbauer Spectroscopic Study
12:30 – 13:00	Šepelák	Local Structural Disorder–Magnetism Relationships in Nanostructured Complex Oxides
13:00 – 14:15	Lunch	
14:30	Excursion	

Wednesday 16.9.		Room 2.005
10:10 – 10:30	Coffee break	
Chair: Guarrotxena		
10:30 – 11:00	Šišková	SERS Detection and Magnetic Removal of Selected Pollutants from Water Using Bimetallic Nanocomposites
11:00 – 11:30	Sunil	Plasmonic Nanoparticles Anchored Electrospun FIbres as Non-Invasive SERS Platforms for Mass Screening of Cancer Biomarkers
11:30 – 12:00	Anucha	Compositional Exploration of Au and Ag Bimetal Alloy Colloids for SERS Detection of Methylene Blue and Chlorpyrifos in Water
12:00 – 12:30	Švecová	Towards Reliable Cu-SERS: Transforming Reactive Copper into Stable Platforms
12:30 – 12:50	Kukralová	Preparation and SERS Utilisation of Chiral Golden Nanoparticles
12:50 – 13:00	NicoletCZ	Molecular spectroscopy from commercial point of view
13:00 – 14:15	Lunch	
14:30	Excursion	

EXCURSION (WEDNESDAY, SEPTEMBER 16)

A guided tour through the historical Olomouc


Olomouc, often referred to as the city with the second-largest historical reserve in the Czech Republic (after Prague), which includes the Holy Trinity Column, a UNESCO World Heritage Site, is definitely worth visiting. Our professional guides will show you the city's highlights and tell you about the history of the second-oldest university in Czechia. In registration form you can choose guide in Czech or in English.

ZOO Olomouc

Zoo Olomouc (Svatý Kopeček, the Holy Hill) is located near Olomouc, Czech Republic, housing over 1,700 animals across 350 species, including unique safari-style exhibits and a 32-meter viewing tower. You will need to get there by public transport. An enthusiastic zoologist will welcome us and guide us through the public and backstage parts of the Zoo, founded in 1952.

Rope centre

If you are up for sports activities during the week full of lectures and scientific discussions, you can enjoy a program in Rope centre Proud called EXPERIENCE, suitable for groups who just want to climb rope obstacles, have fun, and relax from work stress. For those who are afraid of heights, we will find another way to enjoy themselves. You will need to use public transport to reach the rope center.

Thursday 17.9.		Room 2.001	
Chair: Procházka	**8:30 – 9:20**	**Ozaki**	**Advances in Semiconductor SERS**
	9:20 – 9:40	Pěgřimočová	Quantitative Mineralogical Analysis of Sedimentary Rocks Using Far-IR Spectroscopy
	9:40 – 10:00	Horák	MTM – Beyond the Diffraction Limit: Advanced Photothermal Spectroscopy Techniques
	10:00 – 10:20	Tulupová	Combination of SERS and Enzymatic Detection – Introduction of 4D Space for Interference Overcoming
	10:20 – 10:40	Coffee break	
Chair: Šepelák	10:40 – 11:10	Klencsár	Key Insights Into MossWinn 5.0
	11:10 – 11:30	Yaroslavtsev	What's New in Syncmoss – Faster and Smarter Mössbauer Analysis
	11:30 – 11:50	Procházka	Doppler Modulator for Synchotron Mössbauer Spectroscopy
	11:50 – 12:10	Hausner	Observation of Ultrasonically Generated X-Ray Pulses from Resonantly Excited 57-Fe Nuclei
	12:10 – 12:30	Kouřil	Oltwins Tenbeam: A Multi-Beam Mössbauer Spectrometer Towards Higher Efficiency of Measurement
	12:30 – 12:50	Dubiel	Distribution of Cr Atoms in Selected Strained and Strain-Free Fe-Cr Alloys
	13:10 – 14:30	Lunch	
Chair: Holá	14:30 – 15:00	Musil	Photochemical Vapor Generation Coupled with ICP-MS and DART-HRMS: From Highly Sensitive Determination to Volatile Species Identification and Back Again
	15:00 – 15:20	Wahlen	Enhancing Helium Collision and Reaction Cell Modes with A Novel Cell Design for ICP-MS
	15:20 – 15:40	Gregar	Beyond Elemental Certification: Exploring Food CRMs for Nanoparticle Characterization
	15:40 – 16:00	Fouček	Multi-Analytical Spectroscopic Investigation of Roman-Provincial and Germanic Knee Brooches from The Central Danube Region
	16:00 – 16:20	Gibbs	At The Mercy of Sensitivity and Matrix Effects: Quantification of Fluorine and Oxygen in Polymers with Laser-Induced Breakdown Spectroscopy
	16:20 – 16:40	Nyaba	Application of Nickel Iron Layered Double Hydroxides/Activated Carbon (NiFe-LDH@AC) Composite for Preconcentration and Removal of Cr and As from Water Systems
	16:40 – 17:00	Vaculovič	LA-ICP-MS as An Effective Tool for Studying The Fate of Metals in Organisms
	17:00 – 19:00	Optional visit to Fort Science	
	19:00 – 01:00	Conference dinner in Fort Science	

Thursday 17.9.		Room 2.005	
	10:20 – 10:40	Coffee break	
Chair: Schlücker	10:40 – 11:10	Procházka	Beyond Conventional Plasmonics: Next-Generation Materials for Surface-Enhanced Raman Scattering (SERS) Spectroscopy
	11:10 – 11:40	Kočišová	Multifunctional Hybrid Metal Oxide/Metal Platforms for Surface-Enhanced Raman Scattering (SERS): Combining High Sensitivity with Recyclability
	11:40 – 12:10	Dendisová	Electrochemical SERS as A Tool for Studying Molecule-Plasmonic Surface Interactions
	12:10 – 12:40	Kopal	Underestimated Region: High-Order SERS Transitions Reveal Surface Complex Formation
	12:40 – 13:10	Piliarik	Nanoscopic Optical Tracking of The Dynamics of Single Molecules via Elastic and Inelastic Scattering
	13:10 – 14:30	Lunch	
	17:00 – 19:00	Optional visit to Fort Science	
	19:00 – 01:00	Conference dinner in Fort Science	

Friday 18.9.		Room 2.001	
Chair: Šišková	9:00 – 9:30	Guarrotxena	Beyond Single-Analyte Detection: SERS for Multiplexed Biosensing and Bioimaging
	9:30 – 9:50	Pavelka	Spike Annihilator: Life Without Spikes
	9:50 – 10:20	Marques	Advancing Cancer Therapy by Vibrational Spectroscopy – New Drugs and Targets
	10:20 – 10:50	Schünemann	The Mössbauer Effect Can Be Used for More Than Just Detecting The Electronic and Dynamic Properties of Iron Centers in Proteins
	10:50 – 11:00	Closing ceremony	
	11:00 – 11:30	Farewell drink	

CSSC & MSMS SECTION

THE EARLY DEVELOPMENT OF ICP OPTICAL EMISSION SPECTROMETRY IN CZECHOSLOVAKIA: FROM THE FIRST INSTRUMENTS TO MODERN PLASMA SPECTROMETRY

Viktor KANICKÝ

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The introduction of inductively coupled plasma optical emission spectrometry (ICP-OES) into Czechoslovakia in the late 1970s represented a major milestone in the development of modern atomic analytical spectrometry. During the following decades, the technique was gradually adopted by research institutes, universities, industrial laboratories, and governmental organizations, becoming one of the principal methods for multielement analysis.
This lecture presents a historical overview of the early development of ICP-OES in former Czechoslovakia, highlighting pioneering laboratories, the first commercial instruments, and the scientists who contributed to establishing plasma spectrometry in the region. The presentation will also outline the broader evolution of atomic spectrometry, from classical atomic absorption and emission techniques to modern plasma-based analytical methods.
As one example of this development, the lecture will briefly describe the evolution of atomic spectrometry at Masaryk University in Brno, including the establishment of dedicated plasma spectrometry laboratories after 1989 and the current application of laser ablation coupled with ICP-based techniques for direct solid analysis.
By combining historical perspectives with selected examples of present-day instrumentation and applications, the lecture aims to demonstrate the significant development of atomic spectrochemistry over nearly five decades and to document an important chapter in the history of analytical spectroscopy in the Czech Republic and Slovakia.

LA-ICP-MS FOR STRATEGIC RAW MATERIALS: FROM LASER-SAMPLE INTERACTION TO TRACE ELEMENT ANALYSIS, IMAGING AND NEW GLASS CALIBRATION MATERIALS

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Strategic raw materials are essential for low-carbon energy, advanced technologies and secure supply chains. Reliable characterization is crucial for resource evaluation and processing. Li-bearing minerals supply lithium for batteries, whereas U-rich minerals are relevant to nuclear energy and preserve U-Pb records of mineralisation.

LA-ICP-MS provides direct solid sampling, sensitive multi-element analysis, elemental imaging and isotope-ratio measurements. It resolves spatial variations and determines Li, U, associated trace elements and Pb isotope ratios.

Accurate results require control of the entire process from laser-sample interaction and material removal through aerosol generation and transport to plasma, ionization and detection. Matrix, structure, surface condition and laser parameters affect ablation efficiency, elemental fractionation and signal stability.

Reliable quantification also depends on suitable, ideally matrix-matched calibration materials. Because commercial standards for Li- and U-rich minerals are scarce, we develop tailor-made glasses with defined matrix and trace-element contents. Li-rich glasses containing 0.5-5 wt % Li have been characterized by LA-ICP-MS, XRF, µXRF, ICP-OES and ICP-MS methods. The concept is being extended to U/Pb-rich materials, with Pb isotope ratios evaluated by SIMS. Such standards should improve accuracy of in situ analysis of strategic raw materials.

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IMPACT OF MAGNETISM ON LATTICE VIBRATIONS

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According to the standard theory (ST) of the electron-phonon interaction (EPI) the effect of magnetism can be neglected, because the so-called small adiabatic parameter equal to the ratio between the Debye and the Fermi energy is of the order of 10^{-2} [1] and references therein]. However, Kim demonstrated that in systems with itinerant magnetism the impact of the EPI on the spin susceptibility of metals can be enhanced by two orders of magnitude [1]. In other words, the effect of the EPI on magnetic properties of metallic systems, and *vice versa*, is much more important than the ST-prediction. Indeed, based either on recent calculations and/or on measurements results were reported that do not agree with the ST-predictions [2-4].
In this talk I will present experimental results obtained with two techniques viz. (1) ^{57}Fe Mössbauer spectroscopy (MS) on σ-phase Fe-Cr, Fe-V and Fe-Cr-Ni, λ-phase $NbFe_2$ and Fe-As compounds and with ^{119}Sn MS on metallic Cr [5], and (2) nuclear resonant inelastic x-ray scattering (NRIXS) on σ-Fe-Cr (^{57}Fe) [6] and on Cr (^{119}Sn) [7].
A common feature of these systems is delocalized (itinerant) magnetism, hence the Kim's condition for the enhancement of the effect of magnetism on the lattice vibrations. The results clearly demonstrate that the lattice dynamics in the magnetic state of the investigated samples is significantly different than the one in the paramagnetic state. According to the MS-results the vibrations in the magnetic state deviate from the Debye model i.e. they are nonharmonic. The NRIXS study evidences a huge increase of the sound velocity in the magnetic state of the σ-Fe-Cr and an additional mode of vibration in Cr.

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CARBON-ENCAPSULATED Fe_3C NANOPARTICLES FORMED DURING CVD ON AISI 1095 HIGH-CARBON STEEL

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Fe-based substrates are increasingly recognized as active growth media for carbon nanostructures, but the phase state of Fe during growth is often difficult to establish because Fe-bearing domains may remain embedded within a carbon-rich product. Mössbauer spectroscopy is particularly valuable in such systems because it can resolve Fe-specific local environments even when XRD contrast is weak or surface-sensitive methods detect only carbon [1,2]. In this study, carbon nanostructures were synthesized on AISI 1095 high-carbon steel using a two-zone water-assisted chemical vapor deposition process at 800 °C, conceptually following upstream oxygen–hydrogen preheating strategies for in situ water generation [3].
A time-evolution (TEV) series was prepared in the range from 25 s to 120 min. The 90 min growth process was selected for detailed material characterization and examined for substrate-reusability. The ^{57}Fe transmission Mössbauer spectrum of the *TEV-90min* sample shows an Fe-carbide-type environment. Complementary XRD identified carbon structures as the dominant phase with a minor Fe_3C contribution, HR-TEM revealed iron carbide embedded in a carbonaceous matrix, and XPS detected no Fe-related photoelectron signal at the outermost surface.
These results support a model in which water-assisted CVD on AISI 1095 produces a graphitic carbon layer containing buried Fe_3C-like domains that are encapsulated by carbon.

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NANOSTRUCTURED COBALT FERRITE THIN LAYERS PREPARED BY THERMALY INDUCED DECOMPOSITION OF OXALATES

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In this study, we present the preparation and characterization of cobalt ferrites thin-layers doped with selected metal ions in order to modify their functional properties. The controlled growth of oxalate nanostructures from sputtered metal layers, and their thermally induced transformation, allowed the preparation of cobalt ferrite-based thin films with tunable morphology and composition. Several doping strategies were investigated, including the incorporation of manganese to enhance the photocatalytic performance of the materials. Manganese-doped cobalt ferrites are considered promising candidates for photocatalytic applications, especially for the degradation of organic pollutants. [1] The samples characteristics were studied with several techniques: scanning electron microscopy, X-ray powder diffraction and Mössbauer spectroscopy.

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^{57}Fe AND ^{151}Eu MÖSSBAUER AND XRD STUDY OF Eu-DOPED GOETHITE NANO-COMPOSITES PREPARED FROM DIFFERENT Eu-COMPOUND PRECURZORS

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^{57}Fe and ^{151}Eu Mössbauer spectroscopy and powder X-ray diffractometry were used to study Eu-doped goethite ($Eu_xFe_{100-x}OOH$) samples (x = 0, 10, and 30 mol%) synthesized via hydrothermal reaction using starting materials Eu_2O_3, $Eu(NO_3)_3$ and $Fe(NO_3)_3$. Both the as-prepared and thermally treated (300 °C for 30 min) states were studied as potential Na-ion battery anode materials and photocatalysts for water purification. The primary aim was to study the difference in the phase composition of the samples prepared from Eu_2O_3 and $Eu(NO_3)_3$.
^{57}Fe Mössbauer spectroscopy and XRD measurements showed that the hydrothermal reaction produced goethite. The as-prepared and heat-treated $Eu_xFe_{100-x}OOH$ composite systems synthesized from Eu_2O_3 and $Eu(NO_3)_3$ precursors contain different Eu-related phases. XRD patterns show $Eu(OH)_3$ as the main crystalline phase in all samples, while a significant amorphous contribution was also observed. The ^{57}Fe Mössbauer- and XRD results also indicate that the heat treatment leads to complete transformation of goethite into hematite in the composite prepared from the Eu_2O_3 precursor, whereas only partial phase transformation occurs in the $Eu(NO_3)_3$-derived sample. These results also indicate that in the Eu_2O_3-derived sample, part of the goethite is in a paramagnetic state, whereas in the $Eu(NO_3)_3$-derived sample the goethite remains fully antiferromagnetic. This clearly shows that the type of Eu precursor significantly affects the phase composition and the thermal phase transformation. Furthermore, an anomalous modification of the goethite-related reflections was observed in the XRD of the $Eu_{10}Fe_{90}OOH$ composite prepared from the Eu_2O_3 precursor, compared with the undoped sample. This effect can be attributed to Eu incorporation into the goethite structure.
The ^{151}Eu Mössbauer spectra of the 10 mol% Eu samples reflected clear difference between the average hyperfine parameters of the ^{151}Eu Mössbauer spectra in the as-prepared and heat-treated states, in both the oxide- and nitrate-derived systems. This is interpreted in terms of Eu incorporation into goethite.

OPERANDO MÖSSBAUER SPECTROSCOPY FOR SINGLE-ATOM ELECTROCATALYSTS

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Mössbauer spectroscopy relies on recoilless nuclear γ-resonance absorption and features far superior energy resolution compared with XAFS and XPS. Using three hyperfine parameters, namely isomer shift (IS), quadrupole splitting (QS) and magnetic splitting, it enables quantitative and interference-free characterization of single-atom sites of Mössbauer-active isotopes (predominantly ^{57}Fe and ^{119}Sn), including their valence state, spin state, geometric configuration of the first coordination shell, electron density and local electric field gradient. Since the technique exclusively targets specific isotopes, the carbon substrate and doped heteroatoms produce no interfering signals, rendering it ideal for atomic-scale precise characterization of M-N-C single-atom catalysts.

Operando measurement, which acquires spectra synchronously during continuous electrochemical reactions under real applied potentials and electrolyte environments, differs from ex-situ and quasi-in-situ characterizations. It can capture potential-driven reversible structural evolution, spin crossover and transient formation of active metastable states at single-atom sites. This addresses the key bottleneck that the static structure observed ex situ fails to represent the actual active sites during catalysis, filling the gap in dynamic mechanistic characterization for electrocatalysis.

This presentation summarizes the latest research advances, existing technical limitations and future development prospects of operando Mössbauer spectroscopy applied to single-atom electrocatalysts.

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MÖSSBAUER AND COMPLEMENTARY SPECTROSCOPIC STUDIES OF IRON IN FERTILIZERS AND PLANT TISSUES

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Iron (Fe) deficiency represents a significant challenge in agriculture, motivating the development of efficient fertilization strategies ranging from nanotechnology to biodegradable organic complexes. This study utilized ^{57}Fe Mössbauer spectroscopy as a primary analytical tool, complemented by analytical and plant physiological methods, to investigate the synthesis, transformation, and biological availability of two distinct classes of innovative Fe fertilizers. The first part of the research evaluated the potential of ferrihydrite nanoparticles, synthesized with various surfactants, as alternatives to conventional Fe fertilizers [1]. As aqueous ferrihydrite suspensions undergo transformations into more stable, less bioavailable crystalline phases, such as goethite and/or hematite, Mössbauer spectroscopy, accompanied by magnetic measurements and transmission electron microscopy were employed to monitor these structural changes. The second part shifted focus to coordination chemistry, investigating Fe speciation within potential fertilizers prepared with biodegradable lignosulfonate ligands complexed under various pH environments. Mössbauer spectroscopy successfully elucidated the complexation efficiency and chemical stability of the resulting coordination complexes.
To assess biological efficiency, both fertilizer types were evaluated using iron-deficient cucumber (*Cucumis sativus*) as a controlled plant model system to directly compare their biological efficacy. The treatment's success was characterized through X-ray fluorescence mapping, isolated chloroplast Fe quantification and *in vivo* chlorophyll *a* fluorescence induction measurements to monitor the recovery of the photosynthetic apparatus. These physiological experiments on the plant demonstrated how the rate of transformation and the choice of organic material or surfactant directly impact Fe accessibility and uptake by the roots.

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OPTICAL SPECTROSCOPY AND PROPERTIES OF SILICON QUANTUM DOTS

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Silicon quantum dots are a unique material combining low inherent toxicity with typical properties of quantum dots, implying promising application prospects. The problematic feature is that they are in many ways different from well-established binary quantum dots, in terms of both their fabrication methods and higher sensitivity of their electronic structure or photoluminescence response to structural changes due to the covalent bonding nature of their cores. The spectroscopic methods we apply to study this material are not necessarily significantly advanced in their methodology but allow us to arrive at meaningful conclusions about its properties. In particular, we will introduce photoluminescence characterization, showing evidence that ensembles of silicon quantum dots are in most cases made up by dots either bright with ideal near-unity photoluminescence quantum yield, or completely dark [1]. In addition, we will address the structural variability of the surface of silicon quantum dots, which is likely to have implications for quantum dots in general and possibly also for other nanostructures. In nanostructures, the microscopic details of the structural composition inevitably vary from one to another due to surface reconstruction. Silicon quantum dots are an ideal material for the study of such variations, because it exists in a single crystalline phase over a relatively large interval of pressures, significantly simplifying the characterization of structural variability. Moreover, structural variations of the surface can be easily characterized using Fourier-transform infrared spectroscopy, yielding the information on the composition of surface hydrides. The known composition of surface hydrides then let us confirm the possibility of shape-independent surface-facet engineering [2], which significantly impacts chemical reactivity of the produced material. Moreover, implications of the application of an analogical approach to nanodiamonds will be discussed.

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LAYER-BY-LAYER DEFECT ANALYSIS OF HE-ION-IRRADIATED MoS_2

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Defect engineering is a crucial process in the semiconductor industry, and two-dimensional molybdenum disulfide (MoS_2) is an emerging material with promising applications ranging from quantum sensing to single-photon emission. Although irradiation by ions of monolayer MoS_2 has been extensively studied, the characterization and quantification of defects in multilayer two-dimensional materials remain challenging. [1]
Here, we present low-energy He-ion irradiation of a bulk MoS_2 crystal followed by layer-by-layer exfoliation on gold under ultra-high vacuum conditions. This approach enables the preparation of individual layers originating from different depths of the MoS_2 crystal, providing access to the depth evolution of irradiation-induced defects. The exfoliated layers are subsequently analyzed using scanning tunneling microscopy (STM), Raman spectroscopy, and X-ray photoelectron spectroscopy (XPS).
As a direct microscopic method, STM is employed to identify and quantify individual defects, providing a reference for the measurement of defect densities within the top layers of MoS_2. These measurements are further used to calibrate the empirical parameter C(X) in an established Raman model relating the I(LA(M))/I(E_2g) intensity ratio to the defect density. [2] Our results show that Raman spectroscopy provides reliable defect quantification at low defect concentrations, whereas at high concentrations the model no longer applies. On the other hand, XPS appears to be a valuable tool for probing highly defective samples by tracking defect-induced spectral changes in the Mo 3d region.
This work demonstrates a route toward depth-resolved defect engineering in multilayer MoS_2 and provides new insights into the formation and evolution of io n irradiation-induced defects in layered two-dimensional materials.

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MEAN FLUORESCENCE LIFETIME

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The excited-state lifetime is one of the fundamental fluorescence characteristics. It is usually fitted to the multiexponential decay model. However, it is the mean fluorescence lifetime, which enters as an important parameter into numerous calculations characterizing molecular interactions, such as e.g. FRET or fluorescence quenching.
The robustness of the mean fluorescence lifetime toward parameters of the TCSPC (Time-Correlated Single-Photon Counting) experimental setting and mathematical procedures used, will be discussed. Our experiments demonstrated that the intensity-weighted mean fluorescence lifetime is very robust characteristic, in contrast to the amplitude-weighted one, which value is dependent on the data quality and particularly on the used fitting model. A simple method for mean fluorescence lifetime estimation with low computational demands will be presented, which could be a useful tool in the high-throughput applications, such as FACS, FLIM-FRET or HPLC detectors.

EXTENDING AMBIENT MASS SPECTROMETRY USING DEEP-UV LASER–BASED IONIZATION APPROACH

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Ambient mass spectrometry, specifically laser ablation electrospray ionization (LAESI) [1], enables direct chemical analysis under atmospheric conditions without the need for extensive sample preparation, making it highly suitable for rapid and potentially in situ analytical applications. In this work, the capabilities of LAESI are extended by introducing remote deep-ultraviolet (deep-UV) laser-based ionization approach called rDUVLAESCI [2].
The system combines laser-induced deep UV ablation with post-ionization of the generated neutral fine aerosol using a hybrid electrospray ionization–atmospheric pressure chemical ionization (ESI–APCI) environment. A laser beam was used to desorb material directly from the sample surface under ambient conditions. The ablated plume was transferred into the ionization region, where analytes were efficiently ionized via soft ionization processes, minimizing fragmentation and preserving molecular information.
The performance of the developed setup was tested using either spot analysis or mass spectrometry imaging with a focus on the complex real-world sample types. The rDUVLAESCI covered dried spots, latent fingerprints, and cryosections of brain tissue. Fingerprint samples were used to assess trace surface residues containing endogenous lipids and exogenous contaminants, while brain cryosections were employed to evaluate spatially heterogeneous biochemical composition in a complex biological matrix. Across both sample types, signal stability, spectral complexity, and analytical performance under ambient conditions were systematically assessed.

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RAPID SCREENING OF SMALL MOLECULES USING AMBIENT MASS SPECTROMETRY

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Dietary supplements frequently suffer from insufficient quality control, leading to inaccurate label claims or illegal distribution of prohibited substances. The problem of insufficient or even completely absent regulatory control of different supplements spans from poorly regulated natural products containing pharmaceutically active compounds (e.g. lovastatin used for hypercholesterolemia, which can be found in dietary supplements and in EU should be subject of a strict 3 mg daily regulatory limit) to muscle-enhancing compounds such as Selective Androgen Receptor Modulators (SARMs) and anabolic androgenic steroids (AAS) that, despite being completely prohibited, are sold illegally online. Traditional analytical methods for dietary supplements are based on LC-UV-MS/MS. These provide excellent analytical figures of merit, but require 6 to 14 minutes per sample, creating an operational bottleneck for rapid regulatory screening. This study aimed to develop and validate a high-throughput ambient ionization mass spectrometry (AI-MS) method based on Dielectric Barrier Discharge Ionization (DBDI). The primary goal was to achieve rapid screening of small molecules in complex dietary supplement matrices while optimizing the workflow for potential deployment on portable mass spectrometers. Samples – comprising tablets, capsules and liquids – were dissolved in methanol, filtrated and diluted with ultrapure water. To counter matrix effects and signal fluctuations, multiple internal standards were evaluated: lovastatin-d9 for statin profiling, and ostarine-d4, testosterone-d3, and propranolol (utilized as an economical generic standard) for SARMs and AAS analysis. All samples were analyzed using a commercially available Sicrit® DBDI source equipped with a gas chromatography/solid-phase microextraction (GC/SPME) module, coupled to both nominal and high-resolution mass spectrometers (Thermo Scientific Orbitrap Exploris 120 and Agilent 6470A Triple Quadrupole). In order to validate the AI-MS method, an LC-UV-MS/MS assays were developed for each analyte and performed in parallel on the same samples to provide comparative gold-standard reference method. The speed of the analysis is the main advantage of the DBDI mass spectrometry technique, because it is capable of completing sample analysis in just 15 seconds. Because the analysis was targeted or semi-targeted, all the analytes were identified either by extracting specific m/z values to create XIC/EIC chromatograms with a mass accuracy of 5 ppm and better, or by multiple reaction monitoring (MRM). Although the ambient ionization approach exhibited lower linearity and higher signal variability than conventional LC-MS, the normalization using internal standard provided usable calibration. Remarkably, the DBDI method demonstrated a 99.4% qualitative agreement with the reference LC method for identifying illicit substances. Real-sample testing exposed substantial deviations between measured concentrations and manufacturer-declared labels.

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CONCURRENT CHARACTERIZATION OF PLASMONIC HOT SPOT, MOLECULAR STRUCTURE AND MOLECULAR MASS

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Surface-enhanced Raman scattering (SERS) largely relies on the plasmonic substrates. Exact configuration and potentially dynamics of these substrates can play a major role in the overall enhancement. Particularly in the highly enhancing regions known as hot spots [1].
Interferometric scattering microscopy (iSCAT) provides a powerful approach for characterizing the nano-objects and their dynamics directly in solution [2]. When extended with quantitative polarization [3] and phase [4] readout, iSCAT can report on hot spot geometry and the spectral position of the localized surface plasmon resonance. Nanofluidic Scattering Microscopy (NSM) builds on similar interference principle as iSCAT and allows to characterize and/or weigh single nano-objects diffusing in the nanochannel [5].
Hot spot characterization, together with polarization and phase sensitivity, is also central to our recently developed surface-enhanced interferometric scattering (SEiSCAT). This elastic scattering signal is complementary to SERS and shows strong correlation with SERS intensity fluctuations. Moreover, SEiSCAT scales with molecular polarizability, which for similar molecules can be related to molecular mass.
Here, we present concurrent measurements combining polarization- and phase-sensitive iSCAT with down to single-molecule SERS and SEiSCAT readouts. Together, these modalities provide detailed information on hot spot arrangement, surface enhancement, molecular structure, polarizability, and molecular position. As a prospective extension, we envision concurrent measurements of single protein molecules in nanochannels, enabling molecules to be weighed before and/or after they reach the hot spot region.

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THE ROLE OF SURFACE-ADSORBATE BONDING IN SERRS AND IN PLASMON CATALYSIS

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Surface enhanced Raman scattering (SERS) spectroscopy is currently a well-established spectroanalytical tool with a wide range of applications [1]. The 50 years of SERS were celebrated by numerous review articles as well as by the book devoted to both its mechanisms and applications [1]. Surface-enhanced Raman resonance Raman scattering (SERRS) is experienced by chromophoric molecules located at the surfaces of plasmonic metal nanostructures (e.g. Ag nanoparticles, NPs) provided that the excitation wavelength obeys simultaneously the surface plasmon resonance condition for a particular plasmonic nanostructure and the molecular resonance condition for a particular chromophoric surface species. The resulting SERRS enhancement thus originates from both the electromagnetic and the molecular resonance mechanism contributions. Nevertheless, the enhancement factors by these two contributions are not simply multiplicative owing to the resonance damping effect. In our research, we have established the role of surface-adsorbate bonding in the resonance damping effect by revealing that the SERRS enhancement factor for virtually the same chromophore attached to the surface of Ag NPs (assembled into fractal aggregates) by electrostatic bonding is about 500 x larger than for that attached by chemisorption, indicating thus about 500 x lower resonance damping in the former than in the latter case. This result is important for construction of SERRS spectral sensors for biologically and/or analytically important chromophores [2]. Recently, SE(R)RS spectroscopy has been established as an excellent tool for monitoring plasmon-catalyzed reactions undergone by molecules adsorbed on plasmonic metal nanostructured surfaces upon irradiation [1]. Our research on this field has shown that plasmon-catalyzed decarboxylation reactions of $Ru(bpy)_2dcbpy$ and $Ru(dcbpy)_3$ (dcbpy=4,4'-dicarboxy-bipyridine) complexes on Ag NP surfaces proceed entirely under the conditions of chemisorption of these complexes on Ag(0) adsorption sites purposefully generated on the Ag NPs surfaces. The presence of Ag(0) adsorption sites as the necessary condition of the reaction progress is in accord with the charge carriers mechanism of plasmon catalysis, and it can create appropriate conditions for triggering also other chemical transformations plasmon-catalyzed by the charge-carrier mechanism [3].

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SERS-BASED BIOPHOTONICS: FROM NANOTAGS TO LATERAL FLOW ASSAY 2.0

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Surface-enhanced Raman scattering (SERS) is a highly sensitive variant of Raman spectroscopy that exploits tremendous signal enhancement from nanostructures supporting localized surface plasmon resonances (LSPRs). Molecularly functionalized gold nanoparticles, so-called SERS nanotags, can be employed as bright and photostable labelling agents for quantification and multiplexing in biophotonics. Basic considerations on the physics and chemistry of SERS nanotags, including their characterization at the single-particle level by correlative optical and electron microscopy as well as electromagnetic simulations, will be presented. Protein-specific detection is achieved by chemical conjugation of SERS nanotags to target-specific recognition elements such as antibodies to perform immuno-SERS (iSERS). Our vision is to integrate this highly promising iSERS technology into existing work flows of lateral flow assay (LFA) to establish LFA 2.0: a platform that combines the advantages of conventional LFA with the sensitivity of SERS. Our contributions towards achieving this aim also include the development of home-built instrumentation for rapid detection. Finally, current limitations that must be overcome in the future will be highlighted.

MÖSSBAUER SPECTROSCOPY AND MAGNETIC METHODS FOR ENVIRONMENTAL MONITORING IN INDUSTRIAL AND POST-INDUSTRIAL AREAS

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Technogenic magnetic particles (TMPs) emitted during industrial processes accumulate in topsoils and street dusts, forming a sensitive indicator of environmental pollution. Their mineralogical and structural variability reflects technological origin, enabling source identification through combined Mössbauer spectroscopy and magnetic analyses. TMPs from steel metallurgy, coke production, non-ferrous smelting and long-range atmospheric transport were examined to determine iron-bearing phases, magnetite stoichiometry and grain-surface oxidation.

Magnetic parameters, including mass-specific magnetic susceptibility and hysteresis features, differentiated coarse, stoichiometric magnetite typical of iron-metallurgy emissions from fine, defect-rich grains characteristic of Ni–Cu smelter and long-range transported fly-ash sources. Mössbauer spectra decomposition revealed contributions from magnetite grain cores and grain surfaces, maghemite, hematite, goethite and PM aluminosilicates. Grain-size indicators, like Day–Dunlop diagram, confirmed that steel-industry TMPs contain larger PSD–MD magnetite grains, whereas smelter- and long-range-transport-derived particles are dominated by fine, defected and partially oxidized grains with enhanced surface components.

Street-dust analyses showed that fine fractions (<63 μm) are enriched in heavy metals and contain non-stoichiometric magnetite, metallic iron and iron carbides. Strong correlations between magnetic parameters and heavy-metal concentrations demonstrate the usefulness of magnetic screening. A gravimetric microbalance-based susceptometer proved to be an effective low-cost tool for monitoring soils and airborne particles.

The integrated application of Mössbauer, magnetic and gravimetric methods provide a compact framework for identifying TMP sources, assessing pollution intensity and tracking physicochemical transformations of iron phases in industrial environments.

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^{57}Fe-MOSSBAUER STUDY OF PHOTO-FENTON CATALYST PREPARED FROM DOMESTIC WASTE SLAG

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In this study, the relationship between the nanostructure and the photo-Fenton catalytic properties of catalysts derived from domestic waste slag, which is mainly composed of iron-containing soda–lime aluminosilicate, was investigated. The slag was treated with HNO_3 solutions (25, 50, and 75 vol%) and subsequently heat-treated at 800 or 1000 °C for 100 min. Among the prepared samples, the catalyst derived from slag 1807, treated with 50 vol% HNO_3 and heat-treated at 800 °C (designated N50-800-1807), exhibited the highest methylene blue degradation rate constant, reaching 4.70×10^{-2} min^{-1}.

The superior catalytic performance of N50-800-1807 is attributed to its chemical composition, characterized by a basicity (CaO/SiO_2 ratio) of 1.33 and an iron oxide content of 15 mass%, which promoted the formation of tetrahedral $Fe^{IV}O_4$ species and α-Fe_2O_3 nanoparticles. Room-temperature ^{57}Fe Mössbauer spectroscopy revealed a doublet with $\delta = -0.02_{\pm 0.03}$ mm s^{-1} and $\Delta = 1.39_{\pm 0.06}$ mm s^{-1}, assigned to low-spin Fe^{IV} ($S = 1$), together with a sextet with $\delta = 0.42_{\pm 0.04}$ mm s^{-1}, $2\varepsilon = -0.14_{\pm 0.08}$ mm s^{-1}, and $H_{int} = 50.0_{\pm 0.3}$ T, corresponding to α-Fe_2O_3. These species are considered to be the primary active centers responsible for the observed photo-Fenton catalytic activity.

Notably, the low-spin Fe^{IV} species exhibited exceptionally high activity and represents the first experimental confirmation of this oxidation state and spin state in oxide glasses. These findings demonstrate that highly efficient photo-Fenton catalysts for wastewater purification can be produced from domestic waste slag. Furthermore, the results highlight the potential for developing novel functional glass materials through precise control of the oxidation and spin states of transition-metal cations.

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MOLYBDENUM-MODIFIED IRON OXIDES AS CATALYSTS FOR DEGRADATION OF MEROPENEM BY PEROXYDISULFATE

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Meropenem antibiotic is frequently detected in wastewater, however, research on its removal remains limited. The present study introduces molybdenum-modified iron oxides (MFx), synthesized via a solution combustion method, to activate peroxydisulfate (PDS), for enhanced oxidation of meropenem in heterogeneous advanced oxidation processes. The physicochemical and magnetic properties of MFx were systematically analyzed by ^{57}Fe Mössbauer spectroscopy, X-ray powder diffraction, field-emission scanning and transmission electron microscopy, zeta-potential analysis and physisorption (BET) method. The analyses revealed that sodium molybdate and polyvinyl alcohol (PVA) play key roles in forming Mo- incorporated γ-Fe_2O_3. Mössbauer spectroscopy and magnetic characterization further validated the successful incorporation of molybdenum into maghemite. Among the synthesized MFx samples at different iron to molybdenum molar ratios (x), MF 1.0 demonstrated superior catalytic performance due to its higher molybdenum content and larger surface area, achieving >99 % meropenem removal under optimal conditions (0.25 g L^{-1} catalyst dosage, 1.0 mM PDS, pH 4.0). Mechanistic investigations identified sulfate radical ($SO_4^{\bullet-}$) and hydroxyl radical ($HO^{\bullet}$) as primary reactive species, with EPR and XPS measurements confirming the role of Fe^{2+}/Fe^{3+} and Mo^{5+}/Mo^{6+} redox transitions in the activation of PDS. The MF 1.0/PDS system exhibited promising recyclability, maintaining over 90 % meropenem removal efficiency even after five consecutive cycles. The study highlights the potential of molybdenum-modified iron oxides for achieving pharmaceutical remediation, contributing to improved environmental and public health outcomes.

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SPECTROSCOPIC AND PHOTOCATALYTIC STUDY OF β-Fe_2O_3 PREPARED IN THE PRESENCE OF ALKALI CHLORIDES

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This study investigates the properties and photocatalytic behavior of β-Fe_2O_3 prepared through a thermally induced solid-state reaction in the presence of alkali chlorides [1]. β-Fe_2O_3 is a metastable polymorph of iron(III) oxide with structural and optical properties distinct from those of the more common α-Fe_2O_3 phase, making it an interesting material for spectroscopic and photocatalytic studies [2]. The prepared β-Fe_2O_3 samples were characterized using Mössbauer spectroscopy, X-ray diffraction, BET surface area analysis, and scanning electron microscopy to confirm their phase composition and assess differences between materials synthesized with different alkali chlorides. Photocatalytic experiments were carried out using model organic dyes in aqueous solution, and dye degradation was monitored by UV-Vis absorption spectroscopy [3]. This work contributes to a better understanding of how the preparation route influences the properties of β-Fe_2O_3 and its efficiency in light-induced degradation processes.

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LATTICE DYNAMICS AND MAGNETISM OF TWO SIGMA-PHASE FeCrNi COMPOUNDS: MÖSSBAUER SPECTROSCOPIC STUDY

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Two sigma-phase intermetallic compounds viz. $Fe_{50.7}Cr_{46.7}Ni_{2.6}$ and $Fe_{45.8}Cr_{49}Ni_{5.2}$ were studied in the temperature range of 5-295 K by means of Mössbauer spectroscopy. The analysis of the recorded Mössbauer spectra yielded values of average center shifts, <CS>, and relative spectral area, A/A_5. Their temperature dependence revealed an anomalous behavior i.e. a significant decrease of <CS> below ~44 K and ~28 K, respectively, and a big increase of A/A_5 in the same temperature intervals. The anomalies coincide with the magnetic phase in both cases. The maximum decrease of <CS> in the σ-$Fe_{50.7}Cr_{46.7}Ni_{2.6}$ is ~0.02 mm/s what corresponds to an increase of the average square velocity of ^{57}Fe atoms vibrations by ~1.5 $\cdot 10^4$ $(m/s)^2$ or to an increase of the kinetic energy of vibrations by ~2 meV. For the σ-$Fe_{45.8}Cr_{49}Ni_{5.2}$ sample the corresponding figures are ~0.8 $\cdot 10^4$ $(m/s)^2$ and ~1 meV. The largest decrease of the average square amplitude of vibrations amounts to ~$26 \cdot 10^{-24}$ m^2 what is equivalent to the maximum decrease of the potential energy of vibrations by ~13 meV, assuming harmonic vibrations and 155 N/m for the force constant [1]. Analysis of the <*CS*>-data in the paramagnetic phases with reference to the Debye model yielded the value of 415(7) K for the Debye temperature, and that of the A/A_5-data gave 412(16) K. For the σ-$Fe_{45.8}Cr_{49}Ni_{5.2}$ sample, the value of 410(9) K of the Debye temperature of was derived only from the <CS> - data.

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LOCAL STRUCTURAL DISORDER–MAGNETISM RELATIONSHIPS IN NANOSTRUCTURED COMPLEX OXIDES

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The interplay of magnetism and structural disorder in nanostructured complex oxides is a fascinating subject of recent interest [1]. The present work reviews a one-step mechanochemical synthesis and magnetic properties of magnetoceramics with a variety of structure types (cubic spinel, orthorhombic olivine, perovskite, hexagonal structure, double perovskite). The case studies are presented, focusing on recent progress in a fundamental understanding of the structural disorder–magnetism relationships in "interface-controlled" complex oxides prepared by mechanochemical routes. The far-from-equilibrium structural disorder in iron containing magnetic nanomaterials is studied by means of ^{57}Fe Mössbauer nuclear probe spectroscopy. The functional behaviour of mechanochemically synthesized oxides is characterized by SQUID measurements. Selected examples of the separation of interfacial/surface effects from bulk effects in oxide nanoparticles are presented. It is demonstrated that interfacial effects in the mechanochemically synthesized ceramics may result either in an enhancement of magnetic behaviour or in its degradation, *i.e.*, in a desired or undesired magnetic property modification, when compared to magnetism of their bulk counterparts prepared by a conventional ceramic method.

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ADVANCES IN SEMICONDUCTOR SERS

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The SERS enhancement mechanisms of semiconductors are concerned both with electromagnetic and chemical enhancement [1]. 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.
Our group (W. Ji and I) worked on the mechanism and application of semiconductor SERS. Recent our study on semiconductor SERS revealed that Mie resonances scattered near-field effect provided a coherence framework for modeling the electromagnetic mechanism of SERS on semiconductors [2]. We also provided new insights of charge transfer at metal/semiconductor interfaces for hot-electron generation using SERS.
We developed a turn-off SERS sensor for CrO_4^{2-} ions detection in environmental samples using alizarinn red S (ARS)-sensitized colloidal TiO_2 NPs, which was the first attempt to apply semiconductor SERS for quantitative analysis. We also reported two material research based on semiconductor SERS. One was macroscale TiO_2 microspherical arrays with multiple synergistic effect for highly sensitive SERS. Another was bioinspired turing-nanoarchitected needle for solid matrices analysis: a universal platform enabling dual-scale SERS enhancement [3].

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QUANTITATIVE MINERALOGICAL ANALYSIS OF SEDIMENTARY ROCKS USING FAR-IR SPECTROSCOPY

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Knowledge of mineral composition of rocks is essential for both geological exploration and industrial applications. Spectroscopic techniques, such as mid-infrared and Raman spectroscopy, are widely used for analysis of geological samples due to their rapidity and non-destructive nature. Since many sulfide- and oxide-based minerals do not exhibit bands in the mid-IR region, far-IR spectroscopy can serve as a valuable tool for mineralogical analysis, as many inorganic minerals (including those based on oxides and sulfides) exhibit spectral bands in this spectral region [1]. However, the far-infrared spectral region is significantly less utilized in comparison with mid-infrared, primarily due to the challenges related to the development of instruments and use of vacuum or controlled atmospheres during the measurements to avoid the presence of rotational lines of atmospheric water vapor [2,3]. This work evaluates the performance of far-IR spectroscopy for prediction of mineral content in claystones and clay shales. The spectra were acquired without use of vacuum or controlled atmosphere (dry air or nitrogen). Due to the overlap of spectral bands, the multivariate chemometric methods, specifically partial least-squares regression (PLSR), were used. The quantitative data for development of PLSR models were obtained by Rietveld refinement of XRD patterns. In addition, a comparison with mid-IR spectroscopy was made. The study also summarizes the advantages and disadvantages of using various techniques of vibrational spectroscopy for analysis of claystones and clay shales.

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COMBINATION OF SERS AND ENZYMATIC DETECTION - INTRODUCTION OF 4D SPACE FOR INTERFERENCE OVERCOMING

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The development of bio-inspired surface-enhanced Raman spectroscopy (SERS) substrates has emerged as an active area of research in recent years, aiming to provide high analytical performance and low-cost fabrication. On the other hand, one of the more selective and reliable analysis is based on so-called enzyme-assisted analytical chemistry due to the exceptional substrate specificity and catalytic efficiency of enzymes. Enzymatic reactions convert target analytes into measurable products, enabling sensitive and quantitative detection of a wide range of biomolecules, including glucose, lactate, cholesterol, uric acid, amino acids, and other metabolites [1].

However, the main challenge in enzyme-based sensing is the efficient transduction of enzymatic reaction into a measurable analytical signal. Electrochemical detection is the most widely used approach, relying on the measurement of current changes generated by reaction products [2]. Nevertheless, its applicability to complex biological samples is often limited because electroactive species produce interfering signals that reduce analytical selectivity.

Our work demonstrated alternative approach to the integration of SERS and enzymatic reaction for sensitive analyte detection. The general strategy presented involves the fabrication of SERS-active substrates followed by their functionalization with molecules that selectively respond to a specific reaction product generated during an enzymatic process (for example, H_2O_2 or H_2S). Because the concentration of the detected species is directly related to the concentration of the target analyte, the resulting Raman response provides an indirect quantitative measure of the analyte. Compared with conventional approaches, the proposed strategy offers several important advantages, including the time-separation of the enzymatic reaction and detection, cumulative signal measurement, reduced interference from presented molecules, and sensitive analysis of low-volume samples.

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KEY INSIGHTS INTO MOSSWINN 5.0

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Development of the MossWinn program for Mössbauer spectral analysis began in the mid-1990s [1-3]. Originally written in Pascal and compiled with Borland Pascal 7.0 as a DOS protected-mode application, the software underwent a major redesign in the late 2000s to maintain compatibility with contemporary Microsoft Windows systems. This effort culminated in 2010 with the release of the first version in the MossWinn 4.0 series, compiled with CodeGear Delphi 2007 as a native 32-bit Windows executable. Since its introduction as an application software for end users, MossWinn has been maintained through intermittent feature and quality updates distributed via the internet [1]. Several publications have also documented the program's principal capabilities and methodological foundations [2-5].

Development of version 5.0 began in January 2019 by creating a fork of the MossWinn 4.0i codebase within Embarcadero Delphi XE3, with the goal of introducing Unicode support and leveraging the more advanced programming capabilities of this newer environment. The code was subsequently migrated to Embarcadero Delphi 11.3 and, ultimately, to Delphi 12.1.

Version 5.0 constitutes a comprehensive rework of the MossWinn codebase, distinguished in particular by the more extensive adoption of object-oriented design principles in place of the earlier structural programming approach. The new version provides marked gains in performance and overall software quality over version 4.0i, while also adding new capabilities that may substantially improve the efficiency of Mössbauer spectral analysis.

In addition to Unicode support, version 5.0 introduces a range of new developments, among others related to (1) the novel concept of sampled profiles, (2) transmission-integral fitting and analysis capabilities for ^{57}Fe Mössbauer spectra recorded with a synchrotron Mössbauer source, (3) error estimation based on the Monte-Carlo method, (4) new formatted report outputs (xlsx, docx), (5) updated project export/import formats, (6) substantial enhancements to the FIT menu, (7) tools supporting noise filtering and Mössbauer-sample preparation calculations, and (8) the applied physical constants. An overview of the most significant new features will be presented.

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WHAT'S NEW IN SYNCMOSS – FASTER AND SMARTER MÖSSBAUER ANALYSIS

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SYNCmoss is a free and open-source software [1] for fitting ^{57}Fe Mössbauer spectra. Its key idea is that a single, user-friendly GUI handles data obtained by both conventional (laboratory) Mössbauer spectroscopy (CMS) and the Synchrotron Mössbauer Source (SMS) [2], thus, users no longer need to split their work between different programs depending on the technique. The SMS makes feasible experiments that are difficult or impossible with conventional spectroscopy, and it allows the intensity and instrumental-function shape to be tuned for maximum signal-to-noise ratio; this in turn makes determination of the instrumental function essential, since its shape must be accounted for during fitting — especially for high-statistics spectra where instrumental features can be misinterpreted as an extra subspectrum. SYNCmoss extracts the instrumental-function shape from the spectrum of a known absorber and uses the full transmission integral, so the saturation effect is properly included; for CMS the instrumental function is taken to be of Voigt shape with an adjustable width.
The software provides static and dynamic models up to the most general full-Hamiltonian case (for polarized and non-polarized beams), together with multidimensional parameter distributions, correlations and user-defined expressions that let new models be built without touching the source code. It also supports automatic fitting of long spectra series for operando and in-situ studies, and simultaneous fitting of several spectra with linked parameters. Since the initial release a number of features have been added: ● optimization of calculation algorithms ● an interactive plot of the spectrum and its fit; ● a reusable model library that stores fitted models against a given material (mineral, phase, etc.), a small prefilled library of common materials is already implemented and will be enlarged in the future; ● simultaneous fitting of CMS and SMS spectra with parameters linked across the two techniques; ● the MDGD model (multidimensional Gaussian distribution [3]), a more accurate analog of xVBF [4] for correlated hyperfine-parameter distributions; ● an anharmonic spin modulation (ASM) model [5]. More features are planned for upcoming releases. SYNCmoss is now distributed for macOS in addition to Windows and Linux.

New repository is hosted at https://github.com/sergey-yaroslavtsev/syncmoss
The presentation will illustrate the new functionality along with practical fitting examples.

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DOPPER MODULATOR FOR SYNCHROTRON MÖSSBAUER SPECTROSCOPY

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The development of synchrotron radiation sources has also been accompanied by the development of new techniques based on the Mössbauer effect. These techniques include nuclear forward scattering (NFS), nuclear inelastic scattering (NIS), and the more recent synchrotron Mössbauer spectroscopy (SMS). The latter utilizes pure nuclear Bragg scattering on a single crystal of $FeBO_3$ heated to a temperature slightly below the Néel temperature in order to monochromatize the synchrotron beam at the energy of the ^{57}Fe Mössbauer transition to a bandwidth close to 4.8 neV. Thus, when the $FeBO_3$ crystal velocity is modulated with respect to the studied sample, a Mössbauer absorption spectrum can be acquired in energy domain using high-flux synchrotron radiation. However, the tilt of the crystal during Doppler modulation, typically at 12 mm/s, should remain below 0.2 μrad.
We report on the construction of a low-tilt Doppler modulation system dedicated to SMS or other applications requiring low-tilt motion.
The system is based on two high-load, double-loudspeaker-based linear motors. Both motors are mounted on a single mechanical platform placed on a foam support. The first motor is dedicated to moving the furnace with the $FeBO_3$ crystal. During Doppler modulation, due to the conservation laws of momentum and angular momentum, the body of the linear motor moves with respect to the laboratory frame, and the rider (moving platform) also tilts. This movement and tilt are compensated by the second linear motor, which is driven by a signal proportional to the tilt and moves in the opposite direction with a time profile that compensates for both the motion of the first motor and the tilt of the rider.
The system exhibits tilt stability with respect to the laboratory frame below 0.05 μrad while the rider moves with a triangular velocity profile in the range of ±20 mm/s.

OBSERVATION OF ULTRASONICALLY GENERATED X-RAY PULSES FROM RESONANTLY EXCITED 57-Fe NUCLEI

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This presentation reports on the formation and detection of X-ray pulses arising from nuclear resonant excitation and internal conversion in ^{57}Fe Mössbauer absorbers. Unlike transmitted γ-ray pulses, whose temporal profiles are strongly affected by interference between the incident and forward-scattered radiation, the time dependence of X-ray emission is governed by the decay of the excited nuclear state. The X-ray and transmitted γ-ray pulses therefore provide complementary information about the resonant excitation dynamics.
Two situations are investigated: (I) X-ray emission from an ultrasonically vibrating absorber irradiated by a radioactive γ-ray source, and (II) X-ray emission from a stationary absorber irradiated by a γ-ray pulse sequence generated by resonant scattering from an ultrasonically vibrating absorber, as shown in Figure 1. In the first case, the temporal profile of the detected X-ray signal reflects the absorber motion, whereas in the second case it follows the temporal profile of the incident γ-ray pulse sequence. The latter correspondence enables indirect detection of shaped γ-ray pulses through X-ray emission.
Both situations are described theoretically using a one-dimensional quantum-mechanical model and investigated experimentally using a time-coincidence setup. In both cases, the arrival time of the detected X-ray photon is measured relative to a periodically generated start signal synchronized with the ultrasonic vibrations. The results demonstrate that X-ray detection can extend studies of Mössbauer absorber motion beyond conventional transmission geometry. Furthermore, theoretical analysis indicates that magnetically oriented absorbers may enable polarization-selective detection of γ-ray pulses through X-ray emission.

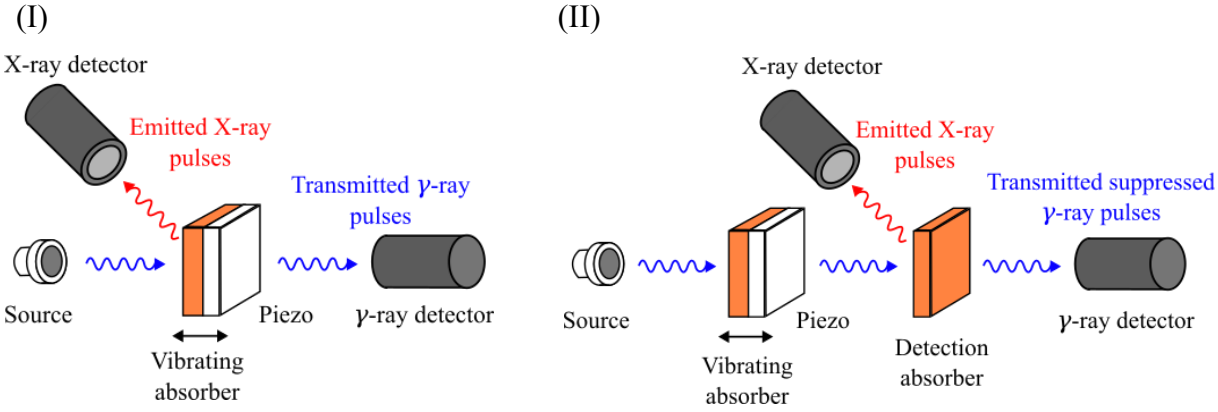

Figure 1: Experimental arrangements for generating X-ray pulses. Left: X-ray emission from a vibrating absorber irradiated by a radioactive γ-ray source. Right: X-ray emission from a stationary absorber irradiated by a γ-ray pulse sequence generated by resonant scattering from a vibrating absorber.

OLTWINS TENBEAM: A MULTI-BEAM MÖSSBAUER SPECTROMETER TOWARDS HIGHER EFFICIENCY OF MEASUREMENT

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Conventional Mössbauer instruments consist of a single velocity transducer with a radioactive source, which irradiates one sample-detector arrangement; therefore, statistically reliable spectra accumulation may require many hours or even days, especially for low iron containing samples, low-activity sources or systematic large sample series studies. This contribution presents the OLTWINS TenBeam concept (a multi-beam Mössbauer spectrometer), which overcomes this limitation by parallel data acquisition around a single radiation source ^{57}Co. The major innovation is an inverse spectrometer geometry. Instead of moving the radioactive source, it is firmly fixed inside a robust lead-shielded central unit, while samples and detectors are mounted on independently controlled velocity transducers. Hence a key technical challenge is the need to move detector-sample assemblies that are considerably heavier than a conventional Mössbauer source. For this purpose, unique high-load electromechanical transducers were developed. Up to ten beamlines can be arranged radially around the radiation source, which enables simultaneous multiple spectra accumulation using the one radiation source. This design increases effective experimental photons utilization, which are emitted from the single radiation source. Moreover, this setup also improves operational safety, as the radiation source remains stationary and shielded during sample exchange or another reconfiguration. The combination of the radial layout with the developed transducers further allows installation of various detector types (scintillation detectors or proportional gas counters) supporting flexible combinations of transmitted gamma rays, conversion electron and conversion X-rays detection.
Performance was evaluated using calibration measurements on standard α-Fe foil at room temperature. Both velocity scale and spectral resolution confirmed that the high moving mass does not affect spectrometer quality; the relative non-linearity remained below 0.1%, which is comparable with standard source moving systems. As a result, ten samples can be measured parallelly in approximately the time, which is generally required to measure only one spectrum. Thus, the OLTWINS TenBeam spectrometer provides a practical route to high-volume Mössbauer analysis and complementary surface/bulk studies for mineralogical, nanomaterial, corrosion, pigment catalyst, and quality-control applications.

Acknowledgements
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DISTRIBUTION of Cr ATOMS in SELECTED STRAINED and STRAIN-FREE Fe-Cr ALLOYS

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Two sets of $Fe_{100-x}Cr_x$ alloys with x=4.85. 12.7, 26.3 and 45.5 were investigated with Mössbauer spectroscopy aimed at revealing an effect of strain on a distribution of Cr atoms. One set was constituted by cold-rolled (CR) or strained alloys and the other one by strain-free (SF) ones. The Mössbauer spectra, recorded at room temperature, were analyzed in terms of two methods: (A) hyperfine field distribution and (B) two-shell model. Results obtained based on A and B gave clear evidence that the Cr atoms distribution in the CR samples was very different than the one in the SF alloys. The difference depends on the content of Cr, and for x=4.85 it was found to be negligible. However, in other SF samples a significant reduction of the Cr atoms number within the first two neighbor shells around the Fe atoms was revealed. This resulted in an increase of the average value of the hyperfine field. The effect was stronger for Cr atoms present in the 2NN shell. Furthermore, it was found that the distribution of Cr atoms in the studied samples is, in general, not random. The departure from the randomness depends on the Cr content, it is characteristic of the neighbor shell and also depends on strain. More details on the issue can be found elsewhere. [1]

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PHOTOCHEMICAL VAPOR GENERATION COUPLED WITH ICP-MS AND DART-HRMS: FROM HIGHLY SENSITIVE DETERMINATION TO VOLATILE SPECIES IDENTIFICATION AND BACK AGAIN

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Photochemical vapor generation (PVG) is an emerging alternative sample introduction technique for analytical atomic spectrometry, combining advantages of efficient separation of analyte from liquid matrix and significantly higher introduction efficiency than possible with conventional pneumatic nebulization of solutions. Volatile analyte species are synthesized during UV irradiation of an aqueous photochemical medium typically containing low-molar mass carboxylic acids, such as formic acid. Its applicability has gradually been expanded to many transition metals, which produce volatile metal carbonyls. Over the past eight years, our group has made significant contributions to the development of new, highly sensitive PVG-based methods coupled with inductively coupled plasma mass spectrometry (ICP-MS), especially for elements such as Mo, W, Ni, Ru, Ir, Rh, and Re.
This lecture will provide an overview of our recent key PVG studies and our successful attempts to identify photochemically generated volatile Ru, Os, Ir, and Rh carbonyls or carbonyl hydrides using a direct analysis in real time (DART) coupled with high-resolution mass spectrometry (HRMS) with an Orbitrap analyzer [1,2]. Additionally, the feasibility of coupling PVG and DART-HRMS for the sensitive and spectral interference-free W determination will be highlighted and its analytical performance will be compared to that obtained with ICP-MS.

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ENHANCING HELIUM COLLISION AND REACTION CELL MODES WITH A NOVEL CELL DESIGN FOR ICP-MS

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Inductively Coupled Plasma Mass Spectrometry (ICP-MS) is a key analytical technique for trace elemental analysis. Traditionally, the use of collision/reaction cell (CRC) gases such as helium and oxygen has been somewhat element-specific, requiring detailed method development and frequent gas switching to optimize sensitivity and eliminate interferences.
This study examines the effectiveness of an enhanced single helium mode for analyzing all elements, with the aim of simplifying laboratory workflows without compromising analytical performance. Our results show that operating ICP-MS in enhanced collision mode provides reliable interference removal across a broad suite of elements, including those that are traditionally challenging to analyze. The simplicity of this approach significantly reduces method complexity and the wasted instrument time associated with gas switching, thereby improving efficiency and reproducibility in multi-element analysis.
We also introduce a new reaction mode in the CRC, using ambient laboratory air as a safer alternative to bottled oxygen. Experimental data indicate that we can achieve similar levels of interference removal and analytical performance for elements such as sulfur, phosphorus, and arsenic, which typically require oxygen for optimal detection. This further streamlines laboratory operations by eliminating the need for a dedicated oxygen-supply infrastructure.
Together, the enhanced He mode and the new reaction mode on the new Agilent 9500 ICP-MS can transform routine ICP-MS analysis by optimizing simplicity, safety, and cost-effectiveness, thereby making high-quality elemental analysis more accessible across various laboratory settings.

BEYOND ELEMENTAL CERTIFICATION: EXPLORING FOOD CRMs FOR NANOPARTICLE CHARACTERIZATION

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The accurate determination of inorganic nanoparticles (NPs) using single particle ICP-MS (spICP-MS) remains analytically challenging due to the lack of dedicated matrix certified reference materials (CRMs). To address this limitation, this study evaluated the suitability of various existing food and biological CRMs as quality control tools for characterizing metal-containing NPs [1]. A screening of diverse matrices was conducted to identify potential candidates for NP quantification. To assess measurement reproducibility, a bilateral comparison was performed between independent laboratories, which demonstrated robust agreement regarding nanoparticle diameters and size distributions, though it also revealed discrepancies in particle number concentrations. Consequently, the research expanded into a deeper investigation of sample preparation strategies using different extraction protocols, namely two enzymatic and one alkaline approach. Testing these approaches on complex biological matrices showed that the choice of extraction protocol may drastically alter both detected particle sizes and concentrations, reflecting variations in extraction efficiency. Furthermore, incomplete matrix breakdown, chemical background contamination, and structural modifications likely caused by CRM pre-treatments complicated the analysis. Ultimately, these experiments demonstrate that while existing reference materials are highly valuable for harmonizing NP size measurements, the development of more robust, standardized extraction workflows and the support of complementary microscopic techniques are essential for successful future NP certification.

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MULTI-ANALYTICAL SPECTROSCOPIC INVESTIGATION OF ROMAN-PROVINCIAL AND GERMANIC KNEE BROOCHES FROM THE CENTRAL DANUBE REGION

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Knee brooches represent one of the most common categories of archaeological finds dating to the Roman period in the Central Danube region. Their popularity extended across both the Roman provinces and the Germanic Barbaricum, resulting in the production of numerous Roman-provincial and Germanic types. Although these brooches exhibit similar morphological characteristics, it remains unclear whether they were produced using comparable alloys, shared the same raw material sources, or employed similar manufacturing technologies. Addressing these questions requires the integration of archaeological interpretation with advanced multi-analytical methods.

Energy-dispersive X-ray fluorescence (ED-XRF) was employed for the quantitative determination of alloy composition. Manufacturing technologies were investigated through traceological analysis using optical microscopy and a TOOLSCAN laser scanning microscope. The traceological observations were subsequently verified by metallographic examination of the internal structure of selected artefacts. Scanning electron microscopy coupled with energy-dispersive spectroscopy (SEM-EDS) was used to characterize surface treatments, such as tinning and silvering. Inductively coupled plasma quadrupole mass spectrometry (ICP-QMS) was applied to determine trace element concentrations and lead isotope ratios in order to assess the provenance of the raw materials.

The integration of multi-analytical data provides new insights into manufacturing technologies, alloy selection, and the provenance of the raw materials used for knee brooch production. These results contribute to a better understanding of the technological differences and similarities between Roman-provincial and Germanic knee brooches and provide new evidence for reconstructing metalworking traditions and material circulation in the Central Danube region during the Roman period.

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This study was carried out in collaboration with the Institute of Archaeology of the Czech Academy of Sciences, Brno, which generously provided the archaeological material investigated in this work and access to the analytical instrumentation of its laboratories.

AT THE MERCY OF SENSITIVITY AND MATRIX EFFECTS: QUANTIFICATION OF FLUORINE AND OXYGEN IN POLYMERS WITH LASER-INDUCED BREAKDOWN SPECTROSCOPY

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Laser Induced-Breakdown Spectroscopy (LIBS) is a well-established technique for elemental analysis of various different samples and matrices. The comparatively simple and cheap instrumentation as well as the possibility to perform multielemental analysis in a spatially resolved manner with high pixel acquisition rates make LIBS a viable alternative to techniques such as electron probe microanalysis, X-ray fluorescence, or secondary ion-mass spectrometry. Compared to Laser Ablation-Inductively Coupled Plasma-Mass Spectrometry, another elemental analysis technique based on laser sampling, LIBS offers access to non-metals such as H, N, O, and F. However, while it is possible to detect these elements with LIBS, limits of detection are generally not suitable for trace element analysis. Additionally, LIBS suffers from strong matrix effects, considering that in a normal LIBS experiment both ablation and excitation/signal generation are intertwined.

In this contribution, we specifically target the analysis of fluorine and oxygen in polymers with LIBS and present novel approaches for quantification. For fluorine, we discuss the impact of ablation atmosphere pressure on signal intensity and the difficulties related to measuring concentrations close to the limits of detection reported in literature. More precisely, at reduced pressure notable improvements in absolute intensity are observed, while the background is decreased, leading to a boost in signal-to-background ratio. For oxygen, an innovative quantitative approach is presented and applied to commercial, UV-aged polystyrene foil to estimate the oxygen uptake by the polymer during the degradation process. Depth-resolved analysis of samples aged for different amounts of time reveal a saturation of oxygen in a surface-near region. In that context, the proposed concept mainly aims to overcome sensitivity issues related to the polymer matrix.

The presented work provides insights into challenges concerning quantitative polymer analysis with LIBS and serves as a foundation for future investigations dealing with other polymer matrices and analytes (e.g., N, P, S, Cl).

APPLICATION OF NICKEL IRON LAYERED DOUBLE HYDROXIDES/ACTIVATED CARBON (NIFE-LDH@AC) COMPOSITE FOR PRECONCENTRATION AND REMOVAL OF Cr AND As FROM WATER SYSTEMS

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A nickel-iron layered double hydroxides/activated carbon (NiFe-LDH@AC) composite was synthesised via hydrothermal-assisted ultrasonic exfoliation, and its structural properties and morphologies were characterised using various analytical characterization techniques. These include transmission electron microscopy (TEM), scanning electron microscopy coupled with energy dispersive spectroscopy (SEM-EDS), Fourier transform infrared (FT-IR) spectroscopy, Brunauer–Emmett–Teller (BET) and X-ray diffraction (XRD). The material was applied as an adsorbent for preconcentration and removal of As and Cr. The target analytes were quantified using inductively coupled plasma optical emission spectroscopy (ICP-OES). Under the optimal conditions, the preconcentration method was validated with respect to linearity, limits of detection (LOQ), accuracy, limits of quantification (LOQ) and precision. The linear ranges were 0.1–150 µg/L and 0.07–100 µg/L for As and Cr, respectively. The precision was investigated in terms of repeatability and reproducibility. The results were expressed in terms of relative standard deviation (%RSD) and the values were less than 5%. The LOD and LOQ ranged from 0.021–0.031 and 0.1–0.07 µg/L for As and Cr, respectively. Finally, the accuracy was validated by successfully analysing spiked samples and the recoveries ranged from 92.6–99.2%. The adsorbent was then explored for the removal of target analytes and adsorption capacities were 102 mg/g and 92.6 mg/g for As and Cr, respectively. The metal ions adsorption was evaluated using kinetics and isotherm models and the results followed pseudo second-order kinetics and Langmuir isotherms. Finally, the removal efficiency for spiked effluent wastewater samples ranged from 89.7–100%.

LA-ICP-MS AS AN EFFECTIVE TOOL FOR STUDYING THE FATE OF METALS IN ORGANISMS

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Organisms are exposed to a whole range of xenobiotics, which can enter organisms in various ways. Many of these xenobiotics are metals and their species. Their fate in the organism can thus be monitored using element-sensitive methods. Among the most sensitive is the laser ablation method with inductively coupled plasma mass spectrometry (LA-ICP-MS).
The lecture will present two applications of this technique in monitoring xenobiotics in organisms. The first will be the monitoring of metal nanoparticles that enter the organism through the respiratory system and are transported via the bloodstream to other mouse organs (brain, liver, kidneys, etc.).
The second case focuses on nickel and cells. Nickel is widely used in materials such as joint replacements and is released into the body. The influence of nickel-containing solutions on its uptake into different types of cells and its distribution within the cell will be monitored.

BEYONG SINGLE ANALYTE DETECTION: SERS FOR MULTIPLEXED BIOSENSING AND BIOIMAGING

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The increasing demand for multifunctional tools in nanomedicine has highlighted the potential of noble metal nanoparticles (NPs) for combined labeling, imaging, sensing, diagnostics, and therapy. Their surface plasmon resonances, highly dependent on nanoparticle structure and environment, enable enhanced molecular recognition and strong electromagnetic field amplification, underpinning the exceptional sensitivity of surface-enhanced Raman spectroscopy (SERS) for single-molecule detection with high specificity. Plasmonic NPs also support optical imaging through light emission and enable photothermal effects for therapeutic applications.
In proteomics, the need for sensitive detection in complex biological systems has driven the development of SERS-based diagnostic platforms, which combine molecular fingerprinting, high sensitivity, and multiplexing capabilities, particularly when integrated with immunoassays. Advances in NP synthesis, assembly, and functionalization have further expanded their biomedical use.
This work presents progress in the design and application of noble metal nanoparticle systems, with a focus on plasmon-enhanced labeling, imaging, sensing, diagnostics, and therapy.

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SPIKE ANNIHILATOR: LIFE WITHOUT SPIKES

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Spike-like artifacts are a persistent nuisance in many instrumental datasets. In Raman and surface-enhanced Raman spectroscopy (SERS), they are often associated with cosmic-ray events and remain an active topic in spectral preprocessing [1,2], but impulse-like disturbances may also appear in other one-dimensional analytical signals, including fluorescence spectra, electropherograms or chromatograms. Although many of them are visually obvious to a majority of analysts, automated removal remains difficult because spikes are peak-like, may overlap with real analytical signals, appear in clusters, or become ambiguous at low spectral sampling density.

Here we present the current development of **Spike Annihilator**, a morphology-guided workflow for detecting and correcting spike-like artifacts, demonstrated on Raman mapping data and electropherograms. This workflow is motivated by earlier experience with mathematical morphology in Raman/SERS signal processing [3] but is now focused also on difficult despiking cases. Candidate events are located using local morphological descriptors and subsequently classified by largely independent shape-sensitive metrics comparing spike-like artifacts with meaningful spectral features. Dataset-level consistency may serve as a fail-safe, but the method does not require repeated acquisition or a clean neighboring spectrum.

Preliminary tests on Raman/SERS data and capillary electrophoresis electropherograms indicate removal of diverse spike morphologies while preserving relevant analytical features. The workflow will be demonstrated on Raman mapping of solid samples acquired using different excitation wavelengths and gratings. The correction is local and conservative: only regions classified as artifacts are replaced, while the remaining signal profile is left unchanged. The broader aim is to provide an open tool for robust despiking of various one-dimensional analytical signals.

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ADVANCING CANCER THERAPY BY VIBRATIONAL SPECTROSCOPY NEW DRUGS AND TARGETS

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Improved chemotherapeutic strategies are an urgent clinical need, since cancer is still the second leading cause of death worldwide, with an expected rising incidence. Metallodrugs developed upon the discovery of cisplatin (*cis*-$(NH_3)_2PtCl_2$) aim at coupling an enhanced efficacy to decreased acquired resistance and harmful side effects. These encompass Pt- and Pd-complexes with more than one metal centre [1], extensively studied by the authors in the last decade [2-7], which trigger a selective DNA damage *via* either metal coordination to the purine bases or electrostatic interaction with the phosphate groups. The design of improved anticancer drugs relies on a thorough understanding of the processes underlying normal-to-cancer transition (NTC), which is still an ill-understood process. Since NTC is closely associated to cellular biomechanical properties, intracellular water has been investigated as a potential drug target [2,6].

Inelastic and quasi-elastic neutron scattering techniques (INS and QENS), combined with Raman and Fourier Transform Infrared (FTIR, including with synchrotron radiation) spectroscopies, were applied to deliver a comprehensive set of data, at the conformational and dynamic levels, on: (i) NTC transformation [7]; (ii) activity of newly developed Pt/Pd-anticancer agents (on DNA, glutathione, proteins, cellular metabolism and intracellular water) [4-6]. Variations in the dynamical profile of intracellular water were unveiled for malignant cells/tissues as compared to healthy ones. In addition, clearly distinct effects were revealed for Pt- *vs* Pd-agents regarding their impact on either the cellular cytoplasm or hydration water in cancer cells, as well as concerning their specific interactions with biomolecules.

This is a pioneer study on the impact of cisplatin-like agents on vital cellular components, which is key for a thorough understanding of their molecular basis of cytotoxicity. These results are expected to foster the development of improved anticancer drugs, displaying high specificity and optimised efficacy, thus contributing to a better prognosis of cancer patients.

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THE MÖßBAUER EFFECT CAN BE USED FOR MORE THAN JUST DETECTING THE ELECTRONIC AND DYNAMIC PROPERTIES OF IRON CENTERS IN PROTEINS

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In this contribution we demonstrate that the ^{57}Fe nucleus can be used to detect electronic and vibrational features in biological systems which may, but do not necessarily, be related to the iron center itself. The first part of this contribution deals with a heme protein which transports nitric oxide (NO). The nitrophorins (NPs) are found in the salivary glands of the blood-sucking kissing bug *Rhodnius prolixus* and have stable ferric heme Fe-NO complexes. The insects use the NPs to transport the signaling molecule NO. Nuclear inelastic scattering (NIS) with an experimental resolution of 8 cm^{-1} of NPs bound to NO detect a strong structured vibrational band at around 600 cm^{-1}, which is due to modes with significant Fe-NO bending and stretching contribution [1]. Based on simulations combining quantum mechanical (QM) density functional theory and molecular mechanics (MM), we demonstrated that protonation of the heme carboxyl groups influences the vibrational properties of the Fe-NO entity. Moreover, heme protonation causes a significant increase of the HOMO-LUMO gap by almost one order of magnitude leading to a stabilization of the Fe-NO bond. In addition, recent NIS experiments on the NO bound form of NP from *Cimex lectarius* with an experimental resolution of ~0.8 cm^{-1} using the Spectrograph at beamline ID14 of ESRF will be presented. Our experiments identify low frequency harmonic protein modes down to about 7 cm^{-1}. In the second part of this presentation, very recent NIS experiments on the iron-sulfur Rieske protein from *Thermus thermophilus* will be discussed. Rieske proteins [2] serve as electron shuttles between other proteins, e.g. in the protein machinery of our cells which is responsible for cell respiration. First QM/MM simulations of our NIS data indicate the presence of collective vibrational protein modes which might play a role in the electron transfer process mediated by the Rieske proteins.

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MICROSYMPOSIUM SECTION

NOVEL PHYSICOCHEMICAL PHENOMENA IN GRAPHENE REVEALED BY MICRODROPLET IN-SITU RAMAN SPECTROELECTROCHEMISTRY

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We introduce a microdroplet in-situ Raman spectroelectrochemistry platform that provides localized access to novel phenomena in graphene under controlled electrostatic and electrochemical perturbations. An electrolyte microdroplet defines a micron-scale electrochemical cell on graphene, enabling us to address a well-defined basal-plane or defect-rich region while simultaneously reading out charge doping, strain, and defect formation with micrometer spatial resolution—capabilities unavailable in conventional, macroscopic spectroelectrochemistry that averages over large, heterogeneous areas.

Using this localized approach, we introduce, for the first time, spectroelectrochemical identification of basal-plane versus defect-related charge-transfer processes in graphene. By comparing monolayer graphene with controlled defect densities, we resolve two distinct G-band components that coexist within the probed area, corresponding to slower basal-plane and faster defect/edge-mediated charge transfer, and thereby directly reveal the electrochemical heterogeneity that is obscured in macro-cell measurements [1].

We further establish a quantitative picture of electrostatic gating of monolayer graphene by highly concentrated aqueous electrolytes. In the high ionic-strength limit, we show that the ionic type and concentration mainly set the initial doping but have negligible influence on the rate of Fermi-level tuning with gate voltage, so that a large fraction of the applied potential is efficiently converted into a shift of the Fermi level [2].

Finally, spatially resolved microdroplet gating combined with Raman mapping allows us to visualize the long-range equilibration of the Fermi level in monolayer graphene. A biased microdroplet on otherwise unbiased graphene produces a sharp G-band change at the droplet boundary followed by gradual recovery of the Fermi level over tens of micrometers, without full return to the initial charge state, revealing graphene's inefficient electrostatic screening and remote gating effects that again extend far beyond the nominally addressed region [3].

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UHV EXFOLIATION AND SPECTROSCOPY OF 2D MATERIALS

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Two-dimensional (2D) materials represent the ultimate limit of vertical miniaturization, providing access to a wide range of unique electronic, optical, and quantum phenomena. Their exceptional properties have attracted considerable interest for both fundamental research and emerging technologies. However, the scalable production of high-quality monolayers remains a major challenge due to the lack of reliable synthesis and manipulation techniques.
Here, we present a facile approach for obtaining bulk-crystal-sized 2D monolayers with nearly 100% yield under ultra-high vacuum (UHV) conditions. Using MoS_2 exfoliated onto different metal substrates as a model system, vibrational and complementary spectroscopic measurements reveal a strong interaction between the metal substrate and the bottom MoS_2 layer. This interaction induces a pronounced strain field in the topmost layer of the bulk crystal, while the underlying layers remain significantly less strained. The resulting vertical strain gradient weakens the interlayer van der Waals coupling, enabling highly selective exfoliation of a single monolayer.
Beyond scalable monolayer production, the proposed approach offers a route to isolating air-sensitive 2D materials that are unstable under ambient conditions. In addition, it provides an ideal platform for investigating their intrinsic properties using surface-sensitive spectroscopic techniques under ultraclean conditions.
The functionality of 2D materials can be further tailored by chemical modification. We will also discuss strategies for achieving controlled chemical functionalization under vacuum conditions, thereby overcoming the limitations of conventional wet chemical approaches and enabling the preparation of pristine, functionalized 2D materials for fundamental studies and future device applications.

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NEW FRONTIERS IN RAMAN SPECTROSCOPY OF 2D MATERIALS: ISOTOPE ENGINEERING AND TWISTED LIGHT

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Raman spectroscopy has become one of the key techniques for investigating two-dimensional (2D) materials, providing detailed insight into lattice dynamics, strain, doping, and interlayer coupling. Recent advances, however, demonstrate that inelastic light-matter interaction is evolving beyond a characterization tool into a versatile platform for studying and engineering novel physical phenomena.
This lecture will present two emerging research directions. The first focuses on isotope engineering, where controlled isotopic substitution enables tuning of phonon frequencies and thermal properties while preserving the electronic structure. Isotopically engineered crystals provide a unique platform for investigating exciton–phonon coupling, vibrational properties, and interlayer interactions inaccessible in naturally abundant materials [1-3].
The second part introduces structured light carrying orbital angular momentum (OAM) as a new degree of freedom in optical spectroscopies on 2D materials [4]. Twisted light possesses a helical wavefront that enables symmetry-selective light–matter interactions and opens new possibilities for probing and controlling low-dimensional (quantum) materials [4, 5].
Selected examples from our recent work will demonstrate how isotope engineering and twisted light expand the capabilities of Raman spectroscopy under ambient as well as extreme experimental conditions, including low temperatures and high magnetic fields.

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TOWARDS ROBUST QUANTITATIVE RAMAN SPECTROSCOPY: FROM FINGERPRINTS TO THERMODYNAMICS

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Raman and Raman optical activity (ROA) spectroscopies are well-established analytical techniques for molecular identification and for conformational and structural characterization of complex molecules. However, obtaining reliable quantitative information from experimental spectra remains challenging, particularly when spectral changes are subtle and occur under varying environmental conditions. Recent advances in Raman metrology have improved data quality, but robust preprocessing is still essential. Reliable solvent subtraction and background correction are often the main limiting factors and have traditionally prevented full automation. As a result, conventional chemometric analyses have usually relied on monitoring intensity changes in a limited number of selected bands.

In this contribution, we show that modern Raman spectroscopy can be extended beyond this conventional approach by treating the entire spectrum as a multidimensional data set. The method is based on a newly developed preprocessing workflow combining singular value decomposition (SVD), asymmetric least squares smoothing (ALS), and iterative feedback. Together with factor analysis and fitting to physico-chemical reaction models, this approach enables the deconvolution of complex spectral series into pure spectral components. Importantly, it also allows reconstruction of spectra of transient or short-lived molecular species that cannot be measured in isolation, such as polyproline I helices at the early stages of mutarotation or specific isolated charge states of nucleotides.

The versatility of this whole-spectrum quantitative approach is demonstrated across different experimental designs. By combining factor analysis with thermodynamic and kinetic modeling of pH, temperature, time, and concentration dependencies, we obtain direct access to fundamental parameters such as pKa values, melting temperatures, kinetic rate constants, and molecular association constants.

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MOLECULAR MATERIALS FOR NONLINEAR OPTICS: AN INTEGRATED APPROACH TO PHASE CHARACTERISATION

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The main motivation for studying molecular materials for nonlinear optics (NLO) is their great potential for technical applications that benefit from numerous NLO effects (e.g., SHG - Second Harmonic Generation, THG - Third Harmonic Generation, and cascaded self-frequency doubling and tripling). These crystalline materials are primarily employed in the generation of new laser frequencies, signal processing, optical communications, all-optical switching, optical power limiting and image manipulation.
Studied molecular crystals are generally formed by highly polarisable organic molecules, which act as carriers of NLO properties, and are hydrogen-bonded in salts and cocrystals containing other inorganic or organic ions/molecules. The presence of hydrogen-bonded cocrystallisation partners enables the crystal engineering of phases with proper crystal packing that fulfil the symmetry conditions necessary for target NLO effects. On the other hand, this bonding mode allows for a wide variety of arrangements of building units with a high probability of phase transitions.
This contribution focuses on the combination of theoretical and experimental methods for phase characterisation and the monitoring of phase transitions in the group of molecular crystals studied, based on guanidine and pyrimidine derivatives. In addition to the combination of crucial temperature-dependent diffraction and, above all, vibrational spectroscopic (IR and Raman) methods, microscopic (polarisation microscopy), calorimetric (DSC), and temperature-dependent SHG studies were successfully employed. Moreover, solid-state DFT computations were also utilised.

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FT-IR SPECTROSCOPY FOR THE NON-INVASIVE ANALYSIS OF PAINTINGS

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FT-IR spectroscopy represents widely used method in the field of heritage science. It is the only available method for non-destructive analysis of binding media in paint layers [1]. Knowledge about binding media is essential to interpret the painting technique used (e.g. oil painting, egg tempera, watercolour etc.). As an indispensable part of a comprehensive assessment of each artwork, it contributes to determining its origin and distinguishing between original and secondarily added layers. Among other things, it helps designing a proper restoration procedure. Furthermore, the binder ageing processes can be monitored and, for example, very early stages of saponification (i.e. metal soaps formation as a result of interaction of fatty acids with pigments) can be detected. In the case of highly valued and well-preserved objects, taking microsamples from a painting is impossible necessitating thus a fully non-invasive approach. In such cases, measurements can only be performed in reflection mode making the analysis more difficult compared to the ATR mode, which is frequently applied to microsamples. In addition, the presence of final varnishes makes it impossible to identify the components of underlying colour layers. This makes paintings without a varnish, such as portrait miniatures or illuminated manuscripts particularly suitable for non-invasive FT-IR spectroscopy set up. Even only with a portable spectrometer very important findings were made. A little oil was found in the binder of miniatures on ivory, although it was originally thought to be pure polysaccharide (watercolour) [2]. It also enabled the detection of thin layer of collodion (a nitrocellulose solution) under the paint and thus allowed to differentiate photographic transfers from genuinely painted miniatures. In the case of medieval manuscripts, non-invasive FTIR spectroscopy is very suitable for investigation of supportive medium (i.e. parchment or cellulose) but also for analysis of pigments and/or binding medium, alternatively.
The aim of this contribution is to demonstrate through practical examples not only the benefits, but also the difficulties and limits of FT-IR spectroscopy in the analysis of cultural heritage objects.

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RAMAN MICROSCOPY OF CRYSTALLINE INCLUSIONS IN MICROALGAE

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Raman microscopy, as an imaging method combining the molecular specificity of vibrational spectroscopy with the spatial resolution of confocal optical microscopy, has proven to be an extremely useful tool for identifying the chemical nature of intracellular organelles and inclusions, as well as for chemical imaging of various microorganisms. Thanks to the methodological progress we contributed to [1], this method could also be used to study photosynthetic unicellular microalgae, where the high autofluorescence of chlorophyll has long been a limiting factor. The use of Raman microscopy has enabled the simultaneous study of intracellular structures such as lipid droplets, polyphosphate bodies, starch grains, mitochondria, and cell walls in intact living cells, in their natural context, without staining or complex preparation. Even more significant was the contribution of Raman microscopy to the reliable identification of the chemical composition of crystalline inclusions, the existence of which had long been known to biologists from polarization or electron microscopy, but the chemical nature of which was unknown or incorrectly determined [2]. Using Raman microscopy, the existence of purine, pyrimidine, and pterin crystals was demonstrated in a wide range of photosynthetic microalgae and other eukaryotic protists [3,4]. Raman microscopy enabled the study of their dynamics and the elucidation of their possible functions. Raman microscopy has thus proven to be an extremely useful tool for studying photosynthetic microorganisms, complementing the ultrastructural information provided by cryogenic electron microscopy and the elemental or isotopic composition information provided by nano-SIMS with unique molecular-chemical contrast. This presentation will also highlight the advantages, perspectives, opportunities, and challenges of the wider use of Raman microscopy in the study of crystalline inclusions, along with its limitations and pitfalls.

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EXPERIMENTAL DEVELOPMENT OF RAMAN OPTICAL ACTIVITY IN OLOMOUC – CELEBRATING 30 YEARS OF ROA IN OUR COUNTRY

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The experimental realization of Raman optical activity (ROA) has undergone considerable technological evolution since its discovery, [1] bringing substantial improvements in signal detection and analytical capabilities [2]. In the Czech Republic, the foundations were laid three decades ago, when the first ROA spectrometer was built and the first experimental and theoretical study of ROA, on α-pinene and *trans*-pinane, was reported [3]. This presentation will provide a personal perspective on several advances of the ROA experiment, including our own contribution at Palacký University Olomouc, where we develop ROA spectrometers for use in research, medical, and industrial applications, in cooperation with the company ZEBR.
A basic, yet potentially very useful application, is the determination of the enantiomeric excess of chiral mixtures, where ROA can achieve accuracies better than 0.1% [4], whilst the detection limit is still far from being reached.
The extended spectral range allows exploration of combinational vibrations [5] and intermolecular interactions in the low wavenumber spectral region [6].
The large variability in polarization modulation [7] is proving very informative. For instance, comparing different modulation schemes can unambiguously distinguish ROA as a single two-photon effect from circularly polarized luminescence (CPL) as two one-photon effects [7].
There is also continued interest in resonance phenomena. It has been demonstrated that resonant ROA (RROA) spectra can be hidden by a signal originating in the interaction between circular dichroism and polarized Raman scattering [8]. Fortunately, this phenomenon can be subtracted, allowing observation of the true RROA, which can be significantly enhanced relative to Raman scattering [9].

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ADVANCED VIBRATIONAL SPECTROSCOPY FOR CHIRAL SOLID-STATE PHARMACEUTICALS

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Solid-state forms of active pharmaceutical ingredients (APIs), such as polymorphs, cocrystals, salts, solvates, and amorphous forms, play a crucial role in modern drug development because they can significantly influence the solubility, stability, dissolution rate, bioavailability, and manufacturability of the API. Therefore, the reliable characterization of these solid forms is essential in pharmaceutical research and production. Vibrational spectroscopic techniques, particularly infrared and Raman spectroscopy, represent fast, inexpensive, and structurally sensitive analytical tools widely used for solid-state characterization. However, closely related crystal forms often exhibit only subtle spectral differences in conventional unpolarized measurements, making reliable discrimination challenging.

In our contribution, we present recent applications of advanced vibrational spectroscopic approaches in the analysis of solid forms of selected APIs. This study combines polarized Raman spectroscopy, vibrational circular dichroism, and density functional theory-based spectral simulations to structurally characterize and distinguish pharmaceutical polymorphs and cocrystals of antiviral and anti-inflammatory drugs [1,2,3]. The results demonstrate that techniques utilizing polarized light provide enhanced sensitivity to crystal packing, intermolecular interactions, and supramolecular organization, enabling the improved differentiation even of closely related solid-state forms, such as diastereomeric cocrystals [4].

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FROM MOLECULAR VIBRATIONS TO CATALYTIC FUNCTION: FTIR SPECTROSCOPY IN ACTION

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Fourier-transform infrared (FTIR) spectroscopy has become an indispensable technique for elucidating reaction mechanisms in heterogeneous catalysis [1-3]. The development of in situ and operando methodologies enables direct identification of active sites, surface intermediates and their dynamic evolution under reaction conditions, providing molecular-level insight into catalytic processes with high temporal and chemical resolution.

Structure–activity relationships in zeolite catalysts are illustrated through representative applications of in situ and operando FTIR spectroscopy. Brønsted acid catalysis in H-ZSM-5 serves as the first example, where FTIR method established the reaction pathway of propene oligomerization by following the formation and evolution of surface carbenium-ion intermediates [1]. Particular attention will be devoted to the influence of proton proximity on reaction kinetics and product selectivity. The discussion then extends to the introduction of redox functionality into zeolite frameworks. Studies of methane activation over iron-containing zeolites demonstrate how time-resolved FTIR spectroscopy, combined with Mössbauer spectroscopy and synchrotron X-ray absorption and diffraction techniques, enables the identification of reactive oxygen species responsible for the selective oxidation of methane to methanol [2]. The final example focuses on bifunctional Fe – and Cu-containing ferrierite catalysts for the direct co-conversion of CO_2 and CH_4 into oxygenates [3]. In situ FTIR spectroscopy reveals the sequential formation of methanol, acetate and acetic acid intermediates, providing direct mechanistic evidence for the cooperative interplay between redox metal centres and Brønsted acid sites.

Together, these examples illustrate how FTIR spectroscopy bridges molecular vibrations with catalytic function across a broad spectrum of catalytic processes—from purely acidic catalysis to redox and bifunctional reaction systems. The integration of operando FTIR spectroscopy with complementary spectroscopic, diffraction and computational methods provide a comprehensive framework for identifying active sites, resolving transient intermediates and establishing reaction mechanisms, thereby enabling the rational design of advanced heterogeneous catalysts.

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NANOSCALE IMAGING AND NANO-FTIR SPECTROSCOPY OF SURFACE NANO-THIN POLYDOPAMINE FILMS – WHAT IS THE ROLE OF DEPOSITION TIME AND SUBSTRATE MATERIAL?

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Polydopamine (PDA) is extensively utilized as an anchoring layer across various applications. Despite its straightforward synthesis, the utility of PDA is constrained by its significant chemical and topological heterogeneity. A comprehensive understanding of the formation process, the physicochemical characteristics of the resulting confluent layers, and the adherent nanoaggregates at the nanoscale is imperative for the expansion of PDA's reliable applications [1]. By employing Scanning Near-Field Infrared Microscopy (SNIM) [2] and nano-FTIR spectroscopy [1], we analyzed PDA layers on three distinct substrates (Si/SiO2, nitrogen-doped TiO2, and Au) at different times of deposition (ToD). Atomic Force Microscopy (AFM) topography was compared with SNIM images acquired at various wavenumbers corresponding to intermediates and polymerization products [2]. Furthermore, a strong correlation has been identified between nano-FTIR and macroscopic FTIR spectra [1, 3], reflecting variations in the relative abundance of PDA and polymerization intermediates. Additionally, the application of principal component analysis (PCA) has yielded further insights by examining loadings, spectral curves, and data distributions in score plots. Notably, spectral variability is greater for ultrathin, confluent surface layers than for nanoaggregates. While the spectra of nanoaggregates exhibited no discernible dependence on ToD or substrate material, the spectra of nanolayers were significantly affected by increasing ToD, suggesting that their growth was influenced by substrate material. At the shortest ToD, spectral clustering based on substrate material indicated a marked influence of substrate material on the physicochemical properties of PDA, an effect that gradually diminished with increasing ToD.

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SERS DETECTION AND MAGNETIC REMOVAL OF SELECTED POLLUTANTS FROM WATER USING BIMETALLIC NANOCOMPOSITES

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Surface enhanced Raman scattering (SERS) spectroscopy has been known for several decades already. Frequently, noble metal nanoparticles and their designed morphologies were successfully used for detection of biomolecules and/or environmental pollutants dissolved at very low concentrations in aqueous solutions [1]. Albeit SERS is frequently regarded as an irreproducible analytical method due to complexity of surface chemistry, it still holds perspective of a robust and reliable analytical tool [2]. When plasmonic nanoparticles are combined into one nanocomposite with magnetic particles, it can be exploited not only for species SERS detection, but also for its permanent removal from aqueous solution due to magnetic field application. This is exactly the main topic of our contribution: indeed, smart polymers containing boronic acid in its structure and/or mercaptophenylboronic acid molecules are attached to plasmonic Au nanoparticles that were generated at the surface of magnetic particles in the previous step. Therefore, bimetallic nanocomposites enveloped by functional surface coating (an organic shell) are employed as SERS-active, magnetically-driven platforms enabling sensitive spectroscopic detection and magnetic separation of selected species. It is challenging task, especially using 785 nm excitation laser line. The successful applicability of bimetallic nanocomposites has been proven in the case of charged porphyrins so far. There is an outlook of selected antibiotics and/or hormones unambiguous spectroscopic detection in aqueous solution via the above-mentioned functional surface modification of our bimetallic nanocomposites.

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PLASMONIC NANOPARTICLES ANCHORED ELECTROSPUN FIBRES AS NON-INVASIVE SERS PLATFORMS FOR MASS SCREENING OF CANCER BIOMARKERS

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Early detection of cancer remains a significant challenge in clinical diagnostics, as many cancers are often identified only after advanced stages [1]. In this context, non-invasive diagnostic strategies based on liquid biopsy have attracted considerable attention because they allow simple and painless sample collection while providing valuable biochemical information relevant to disease detection [2]. The present work explores the development of non-invasive Surface-Enhanced Raman Scattering (SERS) biosensor platforms utilizing plasmonic nanoparticles anchored on electrospun fibers for the label-free detection of cancer biomarkers. The main aim is to establish a reproducible and scalable sensing platform capable of supporting early-stage cancer screening using very small volumes of biological samples. In this approach, electrospun carbon nanofibers functionalized with plasmonic nanoparticles are employed as efficient SERS-active substrates for analyzing salivary biomarkers. The plasmonic nanostructures generate localized electromagnetic hotspots that significantly enhance Raman signals, allowing the detection of trace-level biomolecular signatures present in saliva. The sensing performance of the substrates has been initially assessed using model analytes to verify signal enhancement and reproducibility, after which the platform has been investigated for its ability to distinguish the salivary molecular profiles of cancer patients from those of healthy individuals. The results demonstrate promising sensitivity and classification capability, highlighting the potential of the proposed platform for non-invasive and point-of-care cancer diagnostics. During the talk, we would like to discuss the design and development of these SERS biosensing platforms and key findings from the study will be highlighted. In addition, ongoing research aimed at addressing existing limitations, particularly in terms of sensitivity and analytical reliability, will be discussed, including emerging approaches based on SERS nanotags, which represent an alternative strategy for improving the performance and clinical applicability of SERS-based diagnostic technologies.

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COMPOSITIONAL EXPLORATION OF Au AND Ag BIMETAL ALLOY COLLOIDS FOR SERS DETECTION OF METHYLENE BLUE AND CHLORPYRIFOS IN WATER

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One strategy for expanding SERS substrate materials and morphology generalities for improved detection sensitivity involves the combination (by mole ratio variation) of 2 or more metals to obtain a nano alloy composition [1-3]. In contribution, this study focused Au, Ag, AuAg, and Au_4Ag_6 materials prepared by microwave synthesis for the single metal nano colloids, and galvanic reduction-assisted microwave procedure for the alloyed composition forms. Dynamic light scattering measurement (DLS) showed materials particle size range of 86–152 ± (0.78-3.94) nm. Transmission electron microscopy (TEM) particle size estimation was in the range 61.4 –87.60 ± (15.2–38.3) nm for a revelation of different mix of shape structural morphology. UV-Visible absorption for Au and Ag gave absorption maximum values in line with literature reported data. AuAg, and Au_4Ag_6 materials displayed coherent absorption wavelength values of the individual alloyed elements in the material composition makeup. AuAg and Au_4Ag_6 in comparison to both Au and Ag and for a preliminary test, showed improved SERS performance over the detection of methylene blue (MB), and chlorpyrifos (CPF). AuAg delivered an 0.5 µM LOD for CPF with a correlation constant ($R^2 = 0.96$) and analytical enhancement factor (AEF) of magnitude with 10^4 with respect to the normal Raman measurement. Over MB, Au_4Ag_6 showed a 0.0625 µM LOD at $R^2 = 0.97$ and AEF of $X10^5$ in comparison to normal Raman. Through varying the combination ratio of 2 different metal constituents, we have demonstrated enhanced activity performance of AuAg and Au_4Ag_6 bimetal nano alloy SERS substrates over their single metal analogues at trace level detection of CPF and MB as contaminants of emerging concerns (CECs) in water.

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TOWARDS RELIABLE Cu-SERS: TRANSFORMING REACTIVE COPPER INTO STABLE PLATFORMS

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Copper surfaces offer cost-effective SERS enhancing substrates but suffer from oxidation and corrosion processes. We study strategies for stabilization of Cu surfaces through two approaches: (i) *in-situ* electrochemical modification on Pt/Cu targets [1] using EC-SERS to correlate speciation with performance, and (ii) controlled ageing of Al/Cu substrates [2] to perform long-term studies, stability experiments, and ensure batch reproducibility. Using riboflavin as a probe, we combine multi-scale analyses to identify optimal Cu species and establish a robust protocol for transforming reactive Cu into reliable and stable SERS platforms for analytical applications.

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PREPARATION AND SERS UTILISATION OF CHIRAL GOLDEN NANOPARTICLES

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Chiral nanoparticles represent a fascinating extension of chirality from the molecular scale to the nanoscale, where handedness is no longer limited to molecular structure. Several classes of chiral nanomaterials are currently getting attention, including transition-metal dichalcogenides, quantum dots, perovskite nanostructures, and metallic nanoparticles. Among them, plasmon-active metal nanoparticles, especially gold nanoparticles (AuNPs), are particularly attractive because they combine nanoscale chirality with localized surface plasmon resonances and sub-diffraction electromagnetic field focusing.

This work focuses on the preparation of chiral AuNPs and their utilization as substrates for surface-enhanced Raman spectroscopy (SERS). The combination of chiral response and Raman enhancement provides a platform in which molecules can be detected with high sensitivity while simultaneously retaining information related to molecular handedness. In analytical applications, this opens a route toward enantiomeric detection with limits of conventional SERS and potentially below the concentration ranges of chiral chromatographic methods. Beyond sensing, chiral AuNPs are also promising for catalysis. Importantly, SERS can be used not only as a detection method but also as an in situ spectroscopic probe of reaction intermediates and catalytic efficiency. Chiral AuNPs therefore offer a multifunctional platform connecting plasmonic enhancement, enantiomeric recognition, and reaction monitoring within a single vibrational-spectroscopic approach.

BEYOND CONVENTIONAL PLASMONICS: NEXT-GENERATION MATERIALS FOR SURFACE-ENHANCED RAMAN SCATTERING (SERS) SPECTROSCOPY

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Surface-enhanced Raman scattering (SERS) spectroscopy is a highly sensitive analytical tool for molecular detection and identification. Traditional SERS substrates rely predominantly on noble-metal nanostructures, such as Au, Ag, and Cu, where signal enhancement is mainly governed by the electromagnetic enhancement mechanism. Recently, considerable interest has shifted toward non-plasmonic materials, including metal oxides and conducting polymers, which enhance Raman signals primarily through chemical (charge-transfer) mechanism [1,2]. These materials offer several advantages, such as improved chemical stability, lower fabrication costs, and greater sustainability; nevertheless, their enhancement efficiencies generally remain below those achieved with conventional plasmonic substrates.

Here, plasma-assisted deposition techniques were employed to fabricate hybrid metal–metal oxide (V_2O_5, Ta_2O_5, Nb_2O_5, and WO_3) and metal–polymer (thiophene, quaterthiophene) SERS-active coatings designed to combine the advantages of both enhancement mechanisms. The influence of coating composition and morphology on SERS performance was systematically investigated. The results demonstrate that carefully optimised heterostructures exhibit significantly higher Raman enhancement compared to pure plasmonic, metal oxide, or polymer materials alone. Moreover, certain hybrid systems combining metal oxides with plasmonic Au or Ag exhibit additional photo-induced enhanced Raman scattering (PIERS) effects and UV-induced self-recyclability, thereby offering enhanced multifunctionality. The presented approach offers a promising route toward the development of stable, sensitive, and reusable SERS platforms suitable for advanced analytical and sensing applications.

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MULTIFUNCTIONAL HYBRID METAL OXIDE/METAL PLATFORMS FOR SURFACE-ENHANCED RAMAN SCATTERING (SERS): COMBINING HIGH SENSITIVITY WITH RECYCLABILITY

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Hybrid metal oxide/metal nanomaterials have attracted considerable interest owing to their unique physicochemical properties and multifunctional behavior. One particularly promising application is their use as recyclable substrates for surface-enhanced Raman scattering (SERS)-based detection of biologically relevant molecules. These bifunctional metal oxide/metal systems combine the strong SERS activity of plasmonic metallic nanostructures with the photocatalytic capability of semiconductor oxides [1].
Here, niobium pentoxide (Nb_2O_5) and tungsten trioxide (WO_3) coated with Au and Ag nanostructures prepared by magnetron sputtering were investigated. Using methylene blue (MB) as a model analyte, we show that the SERS enhancement of the metal oxide/metal coatings is dominated by the plasmonic properties of the metallic nanostructures, whereas the metal oxide component plays a key role in photocatalytic degradation under UV irradiation. A faster decrease in the SERS intensity of MB (1×10^{-6} M) was observed for Nb_2O_5/Au nanoparticles compared with WO_3/Au nanoparticles [2]. For Nb_2O_5/Au nanoislands, complete photodegradation of MB proceeded more slowly; however, the substrate retained its ability for repeated regeneration and reuse [3]. In contrast, Nb_2O_5/Ag nanoislands exhibited more efficient surface cleaning, although their long-term reusability was limited. These results demonstrate the critical role of the metal oxide in substrate recyclability and highlight Nb_2O_5-based hybrid platforms as promising candidates for the development of reusable SERS sensors.

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ELECTROCHEMICAL SERS AS A TOOL FOR STUDYING MOLECULE–PLASMONIC SURFACE INTERACTIONS

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Surface-enhanced Raman scattering (SERS) spectroscopy is a powerful technique that enables highly sensitive detection and characterization of molecules located in close proximity to plasmonic nanostructured surfaces. The exceptional sensitivity of SERS originates from two principal enhancement mechanisms. While the electromagnetic contribution has been extensively studied, the chemical enhancement mechanism remains considerably more complex and strongly depends on the physicochemical environment [1].
In this contribution, attention is devoted to investigating the chemical aspects of SERS enhancement using electrochemical SERS (EC-SERS). By controlling the electrode potential, EC-SERS provides a unique opportunity to modulate the processes occurring at the metal surface–electrolyte boundary and monitor dynamic changes in molecular adsorption, and orientation *in-situ*. Experiments were performed using a custom-designed EC-SERS cell developed in-house for integration with an InVia Raman microscope, enabling spectroelectrochemical measurements under well-defined conditions. The capabilities of the method are demonstrated using both model thiol-based [2] systems and selected pharmaceutical compounds from the analgesic family [3].
The study provides deeper insight into the interplay between electrochemical conditions and molecule–surface interactions, contributing to a better understanding of chemical enhancement mechanisms and expanding the applicability of EC-SERS in analytical chemistry, surface science, and pharmaceutical analysis.

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UNDERESTIMATED REGION: HIGH-ORDER SERS TRANSITIONS REVEAL SURFACE COMPLEX FORMATION

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Surface-enhanced Raman scattering (SERS) provides exceptionally rich molecular information; however, most studies focus on the spectral region below 2000 cm^{-1}. As a result, high-order transitions, including overtones and combination bands, remain largely unexplored despite their potential to provide complementary insight into molecule-metal interactions. Here, we demonstrate that these spectral features can serve as sensitive markers of surface complex formation and photon-induced chemical transformations.

As a model system, 4-aminobenzenethiol (4-ABT) adsorbed on highly enhancing silver substrates was investigated using excitation wavelengths of 455, 532, 633, and 780 nm. High-order spectral features were reconstructed from fundamental vibrations, enabling reliable assignment of bands above the conventional SERS range. The results show that these transitions originate from surface-generated 4,4′-dimercaptoazobenzene (4,4´-DMAB) rather than the parent 4-ABT molecule. Their excitation-wavelength dependence reflects differences in dimer-formation efficiency and in molecule-metal surface interactions. Importantly, while combination and overtone bands are typically associated with resonant Raman conditions, their observation in this initially non-resonant system indicates a surface-induced electronic modification of the adsorbed species, consistent with a resonance-enhanced scattering pathway upon complex formation. [1], [2] These findings demonstrate that the spectral region above 2000 cm^{-1} contains chemically specific information commonly neglected in routine SERS analysis.

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NANOSCOPIC OPTICAL TRACKING OF THE DYNAMICS OF SINGLE MOLECULES VIA ELASTIC AND INELASTIC SCATTERING

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Interferometric scattering microscopy is a breakthrough in ultrasensitive, label-free detection of biomolecules enabled by fast and sensitive imaging of light scattered by weakly scattering objects [1]. Our research pushes the boundaries of single-molecule sensitivity and speed focusing on discerning subtle fluctuations in the scattering signal to describe biomolecular interactions and processes hidden deep within the subdiffractional volume of the probe beam [3]. We demonstrate how the fluctuation in the scattering amplitude can be associated with conformation changes taking place at the level of a single, or a few unlabeled biomolecules and open new possibilities for the next generation of super-resolution microscopy techniques [2]. We detect single proteins at microsecond rates and used elastic scattering signal to navigate Raman spectroscopy with single-molecule sensitivity to peak into the structural dynamics of chemical and biochemical compounds [4].

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POSTER SECTION

GREEN SYNTHESIS OF SILVER NANOPARTICLES USING *SARACA ASOCA* LEAF EXTRACT AND THEIR CHARACTERISATION

1

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Environmentally friendly methods for nanoparticle synthesis are increasingly important for developing sustainable nanomaterials. In this study, silver nanoparticles (AgNPs) were synthesised using an aqueous leaf extract of *Saraca asoca* as a green reducing and stabilising agent. The formation of AgNPs was indicated by a colour change from pale yellow to greyish brown, corresponding to the reduction of Ag^+ ions to metallic silver.
The biosynthesised nanoparticles were characterised using UV–Vis, FTIR, XRD, SEM, EDS, and TEM analyses. UV–Vis spectroscopy showed a surface plasmon resonance peak at 425 nm, confirming AgNP formation. FTIR analysis revealed the involvement of phenolic compounds, flavonoids, and proteins in nanoparticle reduction and stabilisation. XRD patterns confirmed the crystalline face-centred cubic structure of metallic silver. SEM and TEM images showed predominantly spherical to quasi-spherical nanoparticles with sizes ranging from 10–50 nm. EDS analysis verified the presence of elemental silver and biomolecule capping on the nanoparticle surface.
The results demonstrate that *S. asoca* leaf extract offers a simple, cost-effective, and eco-friendly route for producing stable and crystalline AgNPs with controlled morphology, making them promising candidates for biological, agricultural, and nanotechnological applications.

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TRIPTYCENE-BASED MOLECULAR MOTORS FOLLOWED BY RAMAN SPECTROSCOPY

2

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The development of two-dimensional (2D) stimuli-responsive systems, consisting of regular arrays of molecular motors, switches, and rotors, is a rapidly growing area of research. These 2D systems, which can reorient or isomerize as a response to external stimuli such as light or electric fields, offer significant potential in molecular nanoelectronics, memory devices, optical filters and heterogeneous catalysis. The characterization of these molecules in solution using various spectroscopic methods including vibrational (particularly Raman) spectroscopy is a relatively well-established process. However, achieving precise control over the positioning of individual molecules on surfaces remains a major challenge. Here, we present a Raman microspectroscopy study of these systems deposited on gold-coated substrates.

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FEASIBILITY STUDY OF COUPLING PHOTOCHEMICAL VAPOR GENERATION AND HIGH RESOLUTION MASS SPECTROMETRY WITH ORBITRAP ANALYZER FOR TUNGSTEN ULTRA-TRACE DETERMINATION

3

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Photochemical vapor generation (PVG) is a sample introduction technique that converts analytes into volatile species under UV irradiation, improving matrix separation and transport efficiency [1]. In our previous work, efficient PVG of W was achieved, enabling ultrasensitive W determination by ICP-MS [1]. High-resolution mass spectrometry (HRMS) with an Orbitrap analyzer provides high mass accuracy and resolving power. Combined with direct analysis in real time (DART), it has recently been used to characterize volatile species generated by PVG [2]. In this work, PVG coupled with DART-HRMS was used to investigate parameters affecting W ion transmission and fragmentation for sensitive W determination.

Instrumental conditions were optimized to favor detection of $MO_xH_y^+$ ions in positive ion mode and $MO_xH_y^-$ ions in negative ion mode. The effects of RF lens voltage and in-source fragmentation on signal-to-noise ratio (SNR) were evaluated. Significantly higher SNR was obtained in negative ion mode. Excessive fragmentation reduced or eliminated CO-containing ions, whereas higher RF lens voltages enhanced signals from major W oxide species. Optimal conditions were 80 V in-source fragmentation and an RF lens voltage of 150%, resulting in the detection of primarily O_3W^-, with the main isotopologues detected between m/z 229.93 and 233.94. Optimization of the m/z range, C-trap ion accumulation time, and number of microscans were also examined to improve SNR. A calibration curve obtained between 0 and 250 ng L^{-1} W showed excellent linearity ($R^2 = 0.9999$). The limit of detection was around 3 ng L^{-1}, limited by blank contamination and comparable to that achieved by ICP-MS [1].

Future work will focus on developing a laboratory-made dielectric barrier discharge (DBD) ionization source to improve ionization efficiency and analytical robustness. This study demonstrates the potential of Orbitrap HRMS coupled with PVG for ultra-trace W determination and future applications in elemental speciation analysis.

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MOBILIZATION OF IODINE FROM SOIL BY METABOLITES OF MICROSCOPIC FILAMENTOUS FUNGI DETERMINED BY ICP-MS

4

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Iodine mobility in soil environments is strongly influenced by interactions with organic and mineral soil components. The aim of this study was to compare the extraction efficiency of metabolites produced by the microscopic filamentous fungi with the sequential extraction of easily mobilizable iodine fractions in a model soil enriched with potassium iodate. A model sample of Chernozem was enriched to a concentration of 10 $mg \cdot kg^{-1}$ iodine and aged for 6 months to simulate iodine redistribution processes in soil. Extraction experiments were performed using fungal metabolites obtained after cultivation in Sabouraud medium. The results showed that fungal metabolites were capable of mobilizing comparable or even higher amounts of iodine than conventional sequential extraction reagents. The obtained results indicate a significant potential of fungal metabolites in mobilizing iodine from soil fractions and their possible application in microbially assisted iodine biofortification of plants. The study further demonstrated that fungal metabolites may affect not only water-soluble and exchangeable iodine forms, but also more stable organically and mineral-bound fractions. Organic acids, redox-active metabolites, and local geochemical changes induced by fungal activity likely play an important role in iodine desorption and mobilization into the soil solution. These findings suggest that fungal metabolites may represent a biologically more relevant model for evaluating iodine availability in soils compared to conventional chemical extraction procedures.

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VIBRATIONAL CHARACTERIZATION OF THE HERBICIDE BENTAZONE: A COMBINED RAMAN AND DFT STUDY

5

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Bentazone is a widely used selective herbicide that frequently leaches into groundwater, raising both environmental and health concerns. Developing reliable, non-destructive analytical methods for its trace detection in aqueous environments is therefore of high importance. In this contribution, we explore the capabilities of Raman spectroscopy combined with quantum chemical calculations for the structural characterization of bentazone under various physicochemical conditions.

We present a comprehensive analysis of bentazone Raman spectra measured in aqueous solutions across varying pH levels and in a series of organic solvents of different polarities. The experimental data reveal distinct spectral markers sensitive to the molecular environment, most notably the significant shift and intensity variations of the carbonyl (C=O) stretching band at 1658 cm^{-1} upon deprotonation.

To rigorously interpret these spectral variations, the experimental findings were combined with advanced density functional theory (DFT) simulations. An extensive conformational analysis identified the stable molecular geometries, which are primarily governed by the torsion of the sulfonyl group and the rotation of the isopropyl substituent. Subsequent frequency calculations, optimally performed at the M06-2X/Def2-TZVPP level using an implicit solvation model, yielded excellent agreement with the experimental data.

This combined experimental and computational approach provides a complete vibrational assignment of the bentazone molecule and elucidates its conformational behavior and protonation states in solutions. These fundamental insights establish a robust spectroscopic fingerprint of bentazone, laying the groundwork for surface-enhanced Raman spectroscopy (SERS) applications aimed at its highly sensitive detection at low concentrations in environmental water samples.

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FORMATION OF GOLD NANOSTRUCTURES MEDIATED BY A NEW FLUORINATED STATISTICAL COPOLYMER

6

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Gold nanoparticles (AuNPs) possessing surface plasmon can be formed by green-chemistry pathways, e.g. using tyrosine as a reducing agent. The presence of a new fluorinated statistical copolymer (FSC) can mediate AuNPs formation under basic environments. Indeed, water-soluble fluorinated polymers have recently emerged, opening a prospective pathway for enhanced imaging based on ^{19}F-MRI (magnetic resonance imaging) [1]. By varying ratios of hydrophilic and fluorinated monomers, the water-solubility of FSC can be adjusted. Moreover, the FSC can be ended by different types of groups containing sulphur to enable efficient conjugation with Au nanostructures (AuNSs). AuNSs can thus represent another imaging modality, optical one, of the prepared nanomaterial serving then as a bimodal imaging tracer which is our aim. Based on the reaction conditions, especially the order of reactants while keeping their molar ratios the same, either plasmonic AuNPs and/or non-plasmonic AuNSs can be formed as revealed in the present study. For the characterization of the as-prepared systems, several spectroscopic and microscopic methods were used: UV-Vis spectroscopy, dynamic light scattering, zeta potential measurements, steady-state fluorescence spectroscopy, Raman spectroscopy, infrared absorption spectroscopy, and transmission electron microscopy (TEM). Based on the results, it can be summarized that fluorescent AuNSs exhibited an emission band with the maximum located at approximately 600 nm when UV excited (280 nm); while plasmonic AuNPs showed an extinction band maximum positioned in the range of approx. 516-530 nm. It was assumed that these AuNPs would be suitable for surface-enhanced Raman spectroscopy, but it was not the case. Nevertheless, the formation of AuNPs was also confirmed by TEM imaging. Instead of SERS-active substrates, the as-prepared plasmonic AuNPs manifested themselves by luminescent features in the near-infrared region (850-950 nm) when 785 nm excitation laser line used. Therefore, they could be exploited as luminescent probes.

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Acknowledgements

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rDUVLAESCI-MS/MSI: A NOVEL APPROACH FOR DIRECT ANALYSIS OF BIOLOGICAL SURFACES AND HIGH-SPEED MASS SPECTROMETRY IMAGING (MSI)

7

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Ambient mass spectrometry has significantly enhanced the insight into the molecular composition of complex biological samples under native conditions, requiring minimal sample preparation [1]. Advancements in laser-based designs, including UV and deep UV lasers, enabled non-destructive, low-fragmentation analysis of various solid samples and dried spots/layers while significantly improving lateral resolution [2] as well as acquisition speed for mass spectrometry imaging (MSI). The presented work introduces a novel, fully automated Remote Deep-Ultraviolet Laser Ablation coupled with Electrospray Ionization−Atmospheric Pressure Chemical Ionization (rDUVLAESCI) ionization source, which can be easily used for either spot analysis or MSI of a wide range of organic molecules with varying polarities and molecular weights.
The rDUVLAESCI-MSI enabled acquisition rate up to 25 pixels/s in a single ionization mode imaging ESI or ESCI and 12,5 pixels/s in simultaneous dual ionization mode imaging. High-quality 2D distribution maps of analytes present in thin mouse brain tissue sections (12-30 µm thick) were successfully displayed with unmatched speed. Among the detected molecules, which are the majority substances in brain tissue, were cholesterol and its derivatives (dehydrocholesterol, oxocholesterol, and desmosterol), free fatty acids (palmitic acid, stearic acid), sphingosine, diacylglycerols (mainly dipalmitoyl glycerol), phospholipids, ceramides and adenine. The promising quantitative potential of rDUVLAESCI-MS has been shown on the linear responses for the brain tissue section with increasing thickness from 12 to 30 µm.
The developed rDUVLAESCI-MS/MSI method represents a fast and versatile approach for direct analysis and MSI of biological surfaces under ambient conditions. The successful highspeed MSI of various lipid-related compounds and small biomolecules in mouse brain tissue demonstrates the ability of rDUVLAESCI-MSI for rapid and detailed molecular imaging of complex biological samples.

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OPTIMIZATION OF ETAAS CONDITIONS FOR LEAD DETERMINATION IN HDES-RS-CPE EXTRACTS

8

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To develop a procedure combining hydrophobic deep eutectic solvent-based rapid synergistic cloud point extraction (HDES-RS-CPE) with electrothermal atomic absorption spectrometry (ETAAS) for the separation, preconcentration, and determination of ultra-trace levels of Pb, it was necessary to optimize both the experimental variables affecting extraction efficiency and the ETAAS measurement conditions. The selected HDES consisted of L-menthol and 1-octanol in a 1:1 molar ratio, while ammonium pyrrolidine dithiocarbamate and Triton X-114 were used as the chelating agent and nonionic surfactant.

In ultra-trace ETAAS analysis, optimization of the temperature program is crucial, particularly for samples containing an organic matrix such as HDES-RS-CPE extracts. The program must ensure complete removal of organic components without analyte loss. The first parameter optimized was the drying temperature; poor control during the second drying step caused evaporation during pyrolysis, leading to smoke formation and reduced reproducibility. A drying temperature of 200 °C provided stable results.

A chemical modifier was also essential, as stable measurements could not be achieved without it. The addition of 2% (w/v) $NH_4H_2PO_4$ was required for both calibration and extract analysis. Reducing the read time to 2.5 s further improved reproducibility.

Pyrolysis and atomization temperatures were optimized using temperature curves for a Pb standard solution (40 µg/L in 0.2% v/v HNO_3) and HDES-RS-CPE extracts in the presence of $NH_4H_2PO_4$. Optimal conditions were 1000 °C for pyrolysis and 1500 °C for atomization, which were applied in the final temperature program for both calibration and sample analysis.

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INVESTIGATION OF INCINERATED SLUDGE FOR SUSTAINABLE PHOSPHORUS RECOVERY USING MÖSSBAUER SPECTROSCOPY

9

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Phosphorus is an essential nutrient for agriculture, but its availability in Europe is limited, resulting in a strong dependence on imports. Also, excessive phosphorus discharge can cause significant environmental problems. One promising approach for phosphorus recovery is the acidic or alkaline wet-chemical treatment of iron containing sewage sludge ash [1]. Sewage sludge ash is the final product of the thermal treatment of digested sewage sludge, and approximately 300,000 tonnes are produced annually in Germany alone [2]. However, wet-chemical recovery processes require large amounts of chemicals. Therefore, further optimization remains an active area of research. This has motivated us to investigate the formation and transformation of iron phosphates throughout different stages of a wastewater treatment plant using Mössbauer spectroscopy. In this way we gain insights into the local chemical environment and speciation of iron-containing compounds. Particular attention is given to the formation of the iron(II) phosphate mineral vivianite formed during anaerobic sludge digestion prior to thermal treatment and to the iron phosphate phases formed during thermal treatment. In addition, laboratory-scale precipitation experiments have been performed to investigate the formation of vivianite under controlled conditions and to compare thermally treated vivianite with thermally treated sewage sludge.

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DETERMINATION OF TOXICITY AND BIOACCUMULATION OF PLATINUM METAL MIXTURES PT AND PD AND THEIR EFFECTS OVER TIME ON SELECTED ORGANISMS OF INDIVIDUAL TROPHIC LEVELS USING THE ICP-MS/MS METHOD

10

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With increasing automobile traffic, the use of platinum metals PTK (Pt, Pd, Rh) is increasing, which are used in automobile catalytic converters. This leads to the release of PTK into the environment and their widespread spread mainly along roads. These PTK can accumulate in living organisms, enter the food chain and adversely affect the vital functions of exposed organisms and can also pose health risks to humans [1].
The toxicity of platinum metals Pt and Pd was tested individually and in a mixture on selected organisms of different trophic levels (green algae *Desmodesmus subspicatus*, mustard *Sinapis alba*). The results show that mustards are less sensitive organisms to PTK, for which approximately the same toxicity was found for Pt and Pd. For green algae, Pd was significantly more toxic than Pt. The results of bioaccumulation studies show the different ability of individual organisms to accumulate platinum metals, which is related to their sensitivity to these metals. The highest bioaccumulation of PTK occurred in mustard, which is the least sensitive to them. The behavior of the organisms themselves is different. The results show higher toxicity of Pt and Pd mixtures for algae compared to the toxicity of individual platinum metals separately and higher toxicity of Pd than Pt. When comparing the toxicity of Pt and Pd, it was observed that approximately the same growth inhibition was caused by significantly lower accumulation of Pd than Pt, therefore we can consider Pd to be a riskier metal for green algae than Pt. In time experiments, the decreasing bioaccumulation and toxicity of individual elements and mixtures over time were monitored. Algae are therefore probably able, unlike mustard, to adapt to increasing concentrations of platinum metals and to engage detoxification mechanisms. Part of the mustard samples were subjected to LIBS analysis. When determining the content of PTK in organisms, we must consider the fact that it is not only the amount accumulated inside the organism, but also the amount adsorbed on their surface.

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IMAGE RECONSTRUCTION STRATEGIES FOR SUBSAMPLED 3D ELEMENTAL MAPPING IN LA-ICP-MS

11

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Laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) enables high-resolution elemental mapping in biological tissues; however, its extension to full three-dimensional (3D) volumetric analysis is limited by extremely long acquisition times. The large number of ablation points required for conventional 3D mapping makes such measurements time-consuming, currently restricting the broader application of true 3D LA-ICP-MS imaging. Consequently, approaches that reduce sampling density while preserving reliable image reconstruction are highly desirable.

This study focuses on reconstruction strategies for recovering 3D elemental distributions from subsampled LA-ICP-MS data. A structured orthogonal subsampling scheme was applied to reduce the number of measured ablation points across volumetric model datasets. Missing information was reconstructed using radial basis function (RBF) interpolation, a mesh-free method suitable for scattered data in multiple dimensions and a flexible alternative to conventional spline-based interpolation.

Two reconstruction strategies were compared using simulated model datasets derived from experimental images of mouse brain tissue. The first approach performs direct 3D reconstruction, in which the sparse volumetric dataset is interpolated as a single 3D RBF model. The second approach decomposes the volume into individual 2D slices, reconstructs each layer independently in the image plane, and subsequently assembles the full 3D volume.

Model data indicate that differences in reconstruction quality are primarily caused by discretization of volumetric information into individual slices during LA-ICP-MS acquisition. Each slice has finite thickness, preventing full continuity along the third spatial dimension. When processed under the assumption of a continuous 3D domain, a mismatch arises between the sampling scheme and the model representation. This leads to systematic artefacts in spatial reconstruction, particularly discontinuities between adjacent layers and increased interpolation error along the Z-axis. As a result, the accuracy of direct 3D reconstruction is reduced, as the stepwise nature of data acquisition and variability between slices cannot be fully compensated by the applied interpolation approaches.

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GREEN SYNTHESIS OF IRON OXIDE NANOPARTICLES USING SPENT MUSHROOM SUBSTRATE OF *PLEUROTUS OSTREATUS*

12

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Iron oxide nanoparticles (IONPs) are widely explored for environmental remediation and catalytic applications, yet conventional synthesis routes often rely on hazardous reagents and energy-intensive conditions. This work presents a green, waste-to-resource approach in which spent mushroom substrate of *Pleurotus ostreatus*, an abundant by-product of edible-mushroom cultivation, serves as the reducing and stabilizing medium. An aqueous extract was prepared from the fungal biomass and combined with iron(III) chloride hexahydrate (FeCl3·6H2O). The reaction pH was adjusted with sodium hydroxide (NaOH) to promote precipitation, and the suspension was stirred to facilitate nanoparticle formation. The resulting product was recovered by centrifugation, washed, and dried to yield a solid powder. Preliminary characterization by UV-Vis spectroscopy indicates the formation of iron oxide nanoparticles. By valorizing fungal biomass that would otherwise be discarded, this approach advances biowaste valorization while avoiding toxic chemical reductants. Planned work will characterize the material's crystallinity, stability, surface charge, and related physicochemical properties to establish structure–property relationships. The study will further explore metal-leaching performance and machine-learning-assisted optimization of the synthesis and application workflow. Together, these efforts position fungal-biomass-derived IONPs as a sustainable platform for environmental and catalytic applications.

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INTERFACIAL ORGANIZATION OF CARBAZOLE-BASED HOLE-SELECTIVE LAYERS IN SILICON SOLAR CELLS PROBED BY MICRO-FTIR AND S-SNIM

13

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Self-assembled molecular interlayers based on phosphonic-acid derivatives have become essential components of high-efficiency silicon solar cells. Among the most widely used materials are carbazole-based molecules such as 2PACz, Br-2EPT, and MeO-4PACz deposited on oxidized ITO surfaces. Despite their successful implementation, the nanoscale organization of these layers remains poorly understood.[1] In particular, it is unclear whether they form well-ordered self-assembled monolayers or exhibit aggregation and/or multilayer formation.
To address this question, oxidized ITO-coated silicon substrates functionalized by laser-assisted deposition of 2PACz, Br-2EPT, and MeO-4PACz are investigated using a combination of micro-Fourier transform infrared spectroscopy (micro-FTIR) and scattering-type scanning near-field infrared microscopy (s-SNIM). Although micro-FTIR provides chemically specific information on the micrometer scale, s-SNIM enables infrared characterization with nanometer-scale spatial resolution, overcoming the diffraction limit of conventional IR spectroscopy. The complementary use of both techniques allows direct assessment of molecular bonding, layer homogeneity, and local structural organization.
The presented approach aims to identify the arrangement of currently employed interfacial molecules and establish spectroscopic markers of ordered and aggregated structures. In future work, the methodology will be extended to newly designed phosphonic-acid-based molecules to evaluate the influence of molecular structure, including π-conjugation, on monolayer formation and interfacial functionality in photovoltaic devices.

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Acknowledgements

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ATMOSPHERE-DRIVEN EVOLUTION OF STEEL POWDERS FOR ADDITIVE MANUFACTURING

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The development of additive and spray-based manufacturing technologies increases the demand for powder feedstocks with controlled phase composition, surface state and deformation behaviour. Stainless and maraging steel powders, represented in this work by CL20ES and CL50WS, are widely used in powder-based additive manufacturing [1]. Their thermal response, however, is strongly affected by annealing atmosphere and temperature, leading to changes in austenite/ferrite stability, oxide formation and particle morphology. These parameters are also relevant for solid-state deposition processes such as cold spray, in which particle bonding is governed primarily by high-velocity impact and severe plastic deformation. For hard, brittle or deformation-resistant powders, controlled pre-treatment by milling and annealing may therefore be necessary to improve deposition behaviour and to support the formation of coherent layered structures.
This contribution combines the study of thermally treated CL20ES and CL50WS steel powders with the development of hybrid CNT-modified steel powder feedstocks. In the first part, phase and structural transformations induced by selected thermal and atmospheric conditions are evaluated by Mössbauer spectroscopy and X-ray diffraction [1], supported by powder metallography, scanning electron microscopy and energy-dispersive spectroscopy. Mössbauer spectroscopy is used as a complementary method for resolving iron-containing phases that may be difficult to distinguish by X-ray diffraction alone, especially in the case of minor or poorly crystalline components. In the second part, carbon nanotubes grown directly on the surface of steel powder particles are considered as a route toward non-conventional steel-carbon nanostructured feedstocks [2,3]. Since CNT-based surface structures may be sensitive to excessive thermal exposure, their integration requires processing routes that preserve their morphology while maintaining suitable powder behaviour for additive or spray-based deposition. The presented approach links phase stability, surface modification and powder morphology as key factors for designing steel-based feedstocks for cold spray and related additive technologies.

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MICROBIALLY DRIVEN CHANGES IN LEAD DISTRIBUTION IN MINE TAILING REVEALED BY SEQUENTIAL EXTRACTION

15

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Sequential extraction is an effective tool for determining the distribution of metals in mine tailings and for assessing how biological processes alter metal speciation and environmental mobility. In this study, the fractionation of lead in flotation waste from the Lintich tailing pond (Banská Štiavnica, Slovakia) was examined to determine how fungal metabolites influence its geochemical distribution and potential bioavailability. The tailing material was subjected to sequential extraction procedure to quantify the distribution of Pb among water-extractable, exchangeable/acid-soluble, reducible, oxidizable and residual fractions. Pb concentrations in all extracts were measured by Flame-AAS (Perkin-Elmer Model 1100, USA) operated under standard conditions for Pb (wavelength 283.3 nm, slit 0.7 nm, deuterium background correction). The method provided a LOQ of 0.05 $mg \cdot L^{-1}$ and calibration range was 0.2 – 20 $mg \cdot L^{-1}$. Subsequently, the material was exposed to adapted and non-adapted strains of *Aspergillus fischeri*, obtained through a gradual adaptation process to the tailing material. The bioextraction experiments were followed by repeated sequential extraction to assess possible redistribution of Pb. The initial fractionation revealed that Pb was predominantly bound to the exchangeable/acid-soluble fraction (>40 %), which indicates a high probability of mobilization. After exposure to fungal metabolites, this fraction decreased significantly to 32.5 % for the non-adapted strain and to 29.9 % for the adapted strain, with a corresponding significant increase in reducible fraction. This shift toward reducible and residual fractions reflects a transition to more stable forms and reduced bioavailability. Overall, the results show that fungal activity not only mobilizes a portion of metals into solution but also induces stabilization processes within the solid phase, effectively lowering the bioavailable Pb fraction. The combined application of bioleaching and sequential extraction thus provides a better understanding of how fungal metabolites affect metal fractionation in mine tailings and influence their environmental risk.

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SUPPRESSION OF NONSPECIFIC SORPTION OF NANOPARTICLE-ANTIBODY CONJUGATE IN P53 PROTEIN DETECTION

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Immunoanalytical techniques are an important tool in disease research and diagnostics. These methods utilize a highly specific interaction between antigen and a labelled antibody. In this work 60nm gold nanoparticles were used as labels and subsequently detected using LA-ICP-MS. Utilization of nanoparticle-antibody conjugates with this detection method increases the sensitivity of the immunoassay. However, it also results in an increase in background signal due to nonspecific interactions. These interactions are caused by hydrophobic attraction, electrostatic attraction, species cross-reactivity etc [1]. Hence optimization of sample preparation is necessary to minimize these effects.
This research is focused on optimizing the dot-blot method for detection of the p53 protein in cellular lysates. The key optimized parameters were membrane material and sample volume. Additionally, the lower limit of the working range of the immunoassay was determined. The work also investigated the underlying causes of the observed effects and led to an improvement of the repeatability of the method.

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POSITIVE GADOLINIUM ANOMALY IN COMMON FOODSTUFFS AS A MARKER OF ANTHROPOGENIC ENVIRONMENTAL CONTAMINATION

17

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Gadolinium is one of the rare earth elements, whose use in industry, medicine, and agriculture has increased significantly in recent decades. An important source of anthropogenic gadolinium (Gd_{anth}) is represented by gadolinium-based contrast agents (GBCAs) widely used in magnetic resonance imaging. After administration, these compounds are excreted largely unchanged and enter aquatic environments through municipal wastewater. Since conventional wastewater treatment plants are not designed to effectively remove rare earth elements, their release and accumulation in the environment continue to increase. Elevated concentrations of gadolinium are reflected by the so-called positive gadolinium anomaly, which is considered a useful indicator of anthropogenic influence on the environment. Although the presence of anthropogenic gadolinium has been repeatedly reported in surface water, groundwater, and drinking water, information on its occurrence in food intended for human consumption remains very limited. Therefore, the aim of this study was to investigate the content of Gd_{anth} in commonly consumed foods originating from Europe and Asia and to evaluate the occurrence of gadolinium anomalies as evidence of anthropogenic environmental contamination [1,2].
Samples of wheat, spelt, and rye flour, rice, and carrots were analyzed. Concentrations of rare earth elements were determined using inductively coupled plasma mass spectrometry. The magnitude of the gadolinium anomaly and the content of anthropogenic gadolinium were estimated from shale-normalized REE concentrations. A positive gadolinium anomaly was detected in most of analysed sample types. Median concentrations of Gd_{anth} ranged from 3.05 to 10.5 $\mu g \cdot kg^{-1}$, with considerable variability among individual samples. The highest concentrations were found in wheat flour, whereas the lowest levels were observed in rice. The results suggest that the content of anthropogenic gadolinium in food may be influenced by irrigation water quality, agricultural practices, and local anthropogenic environmental pressures. The results obtained provide some of the first evidence of anthropogenic gadolinium occurring in commonly available food products. The study confirms the suitability of ICP-MS for monitoring trace concentrations of rare earth elements in food matrices and highlights the need for systematic monitoring of anthropogenic gadolinium in food chains with respect to human health protection and food safety.

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DEVELOPMENT OF THE RAPID LA-ICP-MS METHOD FOR ELEMENTAL MAPPING IN BIOLOGICAL TISSUES

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LA-ICP-MS is an analytical technique enabling spatially resolved determination of elemental distributions in solid samples at the microscopic level and is well suited for imaging and mapping applications in biological tissues due to its high sensitivity and minimal sample preparation requirements. However, its broader application is limited by the time-intensive nature of conventional measurements, resulting in increased analytical costs. In this study, an alternative approach based on quasirandom sampling strategies, such as Halton sequences, combined with Bayesian image reconstruction is proposed to replace traditional orthogonal scanning. For a 1 cm² model sample area and a spatial resolution corresponding to a 100 µm laser spot size, the number of ablation points was reduced from 40,000 (orthogonal grid) to approximately 6,600. This reduction led to a decrease in analysis time of up to 80 %, while also enabling uncertainty quantification of the reconstructed images, allowing identification of poorly reconstructed regions and supporting targeted re-sampling. The quality of reconstructed images obtained in the simulation was evaluated using the Structural Similarity Index Measure (SSIM), yielding a value of 0.66, indicating good agreement with conventionally acquired images with all relevant structures in the sample captured. In a separate experiment on mouse brain tissue sections, an area of 0.5 × 0.2 cm was analysed. Using the conventional approach, an orthogonal grid of 1,000 ablation points was applied, whereas the pseudorandom strategy required only 117 points based on a Halton sequence. The reconstructed image quality, evaluated by SSIM, reached a value of 0.78, indicating good agreement with the corresponding reference image. The proposed methodology significantly accelerates LA-ICP-MS imaging and enhances sample throughput, offering a promising tool for efficient elemental mapping in biological research.

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OPTIMIZATION OF PHOTOCHEMICAL VAPOR GENERATION OF FLUORINE COUPLED WITH INDIRECT DETECTION BY ICP-MS/MS

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Fluorine (F) is environmentally relevant due to its involvement in persistent and toxic organofluorine compounds, but its trace-level determination remains challenging. Direct F detection by Ar-based inductively coupled plasma mass spectrometry (ICP-MS) is inefficient because of poor ionization and severe polyatomic interferences at *m/z* 19. Indirect detection using plasma-formed $[^{138}Ba^{19}F]^+$ by triple quadrupole ICP-MS/MS enables sub-ppm determination of F, but conventional solution nebulization still limits introduction efficiency and matrix tolerance. Photochemical vapor generation (PVG), which converts analytes in solution into volatile species, is a promising alternative for improving introduction efficiency and reducing matrix transport to the plasma. For F, a previous GC-MS work demonstrated fluoromethane (CH_3F) formation from dilute acetic acid with Cu^{2+} as a mediator, but the yield remained low (<1%). Moreover, offline GC-MS detection limited the detailed optimization of PVG conditions. This motivated us to combine PVG with indirect F detection by ICP-MS/MS. The results of this ongoing study will be presented. First, indirect F detection by ICP-MS/MS was optimized using solution nebulization of F and Ba^{2+}, improving the signal-to-background ratio (SBR) of $[^{138}Ba^{19}F]^+$ by approximately 5-fold. The optimized BaF^+ detection strategy was then coupled to a flow-injection (FI) PVG system based on a low-pressure Hg thin-film flow-through photoreactor, enabling online monitoring of transient BaF^+ signals for systematic optimization of PVG conditions. The identity of acid in the liquid medium strongly affected the BaF^+ response. Propionic acid performed best among formic, acetic, and propionic and their mixtures. Cu^{2+} remained the most efficient mediator, with only modest additional enhancement from Cu^{2+}/Mn^{2+} and Cu^{2+}/Fe^{2+} combinations. The addition of mM concentrations of sodium acetate produced a singificant enhancement, suggesting the possible effects of the presence of carboxylate anion and/or the medium pH on PVG of F. Other mediators and additives are currently being evaluated to further optimize the photochemical medium. The results also indicate that irradiation time is critical, but long irradiation times (>90 s) are difficult to achieve in the continuous-flow mode of operation of the thin-film photoreactor. Therefore, a stop-flow mode and coiled tubing reactors will be evaluated to extend the effective irradiation time.

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POSITRON ANNIHILATION SPECTROSCOPY COMPLEX BASED ON CAEN DIGITIZERS

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Positron annihilation spectroscopy (PAS) is a non-destructive method used to detect vacancy defects in a wide range of materials. It is particularly well-suited for investigating the size and concentration of vacancy defects at various depths in metals, alloys, semiconductors, porous materials, and polymers. Two techniques, positron lifetime spectroscopy (PALS) and Doppler broadening spectroscopy (DBS), enable investigation of vacancy-type defects sized below the resolution of transmission electron microscopy. The PAS complex uses LaBr:Ce or BaF_2 scintillation detectors to measure the PALS spectra. Lifetime measurements using ^{22}Na as a positron source are performed using a 14-bit CAEN waveform digitiser (DT5730S) operating at a 500 MHz sampling rate. Data collection and experiment control are performed using the CoMPASS user programme. Since the constant-fraction discriminator (CFD) is the most suitable method for time estimation, the CFD algorithm is applied to the original signal to obtain a bipolar zero-crossing signal for estimating the timestamp. The time resolution represented by FWHM (full width at half maximum) of the time distribution was measured using the coincidence gamma-rays of ^{60}Co (1173 and 1332 keV). The time resolution (FWHM) was 214 ps for the LaBr:Ce detectors. The analysis of the experimental time distribution has been attempted with the PATFIT19 analysis software. For coincidence Doppler broadening spectroscopy (CDBS) were used two HPGe detectors (GCD 30185 from BSI, Riga, Latvia) and CAEN dual digital multichannel analyser (DT5780P), which includes two high-voltage power supplies for HPGe detectors and two built-in multichannel analysers with 16,384 channels. The device was again controlled and operated via the COMPASS user programme. The energy resolution was determined for selected line types (^{152}Eu, ^{137}Cs and ^{60}Co) and the energy resolution for annihilation radiation (511 keV) was estimated to be 1.40 and 1.39 FWHM for the first and second HPGe detectors, respectively. The detectors were synchronised using a digitiser set in coincidence mode. The value of 10 ns was selected as the coincidence window. The experimental data were processed into 2D CDBS spectra using proprietary software.

SURFACE BEHAVIOR OF 1.2709 MARAGING STEEL PRODUCED BY SELECTIVE LASER MELTING – MÖSSBAUER STUDY

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Maraging steel is a high-strength material with enhanced mechanical properties. Mössbauer spectroscopy (MS), also known as recoilless nuclear gamma resonance, can be used to study the surface and bulk of a material. Conversion X-ray Mössbauer spectroscopy (CXMS) and conversion electron Mössbauer spectroscopy (CEMS) provide information about the structure of materials at different depths: 10 μm and 0.3 μm, respectively. This method can reveal information about the inhomogeneity of the material's surface layer.
In this research, the study samples were made from 1.2709 maraging steel metal powder using selective laser melting (SLM). The initial samples were in the shape of a cylinder with 25 mm diameter and 5 mm height. After 3D printing, the surface of the studied samples was subjected to a post-production treatment process. The samples were studied under the following conditions: after sandblasting; after sandblasting and annealing at 500 °C in air, after polishing; and after polishing and annealing at 500 °C in air.
Studies of the phase composition and phase transformations of 1.2709 maraging steel have revealed the relation between surface treatment methods and phase distribution. A detailed investigation of the surface of the sample revealed that the initial sandblasted and polished samples contained martensite and retained austenite phases. The phase composition in the surface layer is also affected by the surface treatment method. While the polished sample showed only the martensitic phase, sandblasting preserved both the austenitic and martensitic phases. The samples exposed to temperature also show the presence of iron oxide (α-Fe_2O_3) at a depth of around 10 μm. Studies of the thin surface layer at depth between 0.1 and 0.4 μm have revealed that the surface is inhomogeneous. A polished surface tends to create the α-Fe_2O_3 oxide when exposed to temperature, whereas a sandblasted surface is covered with γ-Fe_2O_3.

ETV-ICP-OES: A POWERFUL TOOL FOR THE DETERMINATION OF MRI/PET MARKER DISTRIBUTION IN MOUSE TISSUES

22

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Electrothermal vaporization (ETV) coupled with inductively coupled plasma optical emission spectroscopy (ICP-OES) enables rapid multielement analysis of major, minor, and trace elements without pre-treatment of solid and liquid samples, aside from humidity drying. Unlike solution nebulization used in traditional ICP-OES, this approach reduces the risk of sample contamination. Detection limits and the required sample volume/amount (a few milligrams or less) for analysis decrease as the sample aerosol is transported with high efficiency to the ICP torch. Integrating ETV with ICP-OES enables swift, direct, and fully automated analysis of multiple samples using in-house or certified solid and aqueous standards.
We exploited this method to develop a reliable methodology for monitoring the new PET/MRI probe [18F][Gd(FL1)] in tissues [1], specifically assessing the dynamics of Gd/probe distribution in mice. The optimized parameters enable detection from trace levels to ca. 1000 mg/kg (depending on the analytical lines used), with detection limits from 0.01 mg/kg to 4.7 mg/kg and a ca. 5% error of determination. Results matched radioactive labeling assessment, demonstrating ETV ICP-OES's effectiveness.

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INTEGRATING SPECTROSCOPY TO ASSESS COPPER(II) AND ARSENIC(V) UPTAKE BY KEFIR GRAIN BIOSORBENTS

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This study evaluates the potential of kefir grains, a polysaccharide-rich byproduct of beverage fermentation, as sustainable biosorbents for removing copper(II) and arsenic(V) from contaminated water. Although kefir grains have been explored for organic pollutant removal, their application in heavy-metal remediation remains limited. Here, we compare the biosorptive performance of milk and water kefir grains and characterize their metal-binding behavior using flame atomic absorption spectrometry (FAAS) for quantitative metal analysis, scanning electron microscopy (SEM) for surface morphology assessment, and Fourier-transform infrared spectroscopy (FTIR) to identify functional groups involved in adsorption. Milk kefir grains exhibited significantly higher sorption efficiency, removing up to 95% of copper(II) at low concentrations (0.16 $mmol \cdot L^{-1}$) with a maximum sorption capacity of 49 $\mu mol \cdot g^{-1}$, compared to 35.5% removal by water kefir grains. For arsenic(V), milk kefir grains achieved 56% removal with capacities up to 20 $\mu mol \cdot g^{-1}$, again outperforming water kefir grains (34.5% maximum removal). Spectroscopic analyses confirmed distinct structural and functional-group differences influencing sorption behavior. Overall, kefir grains, particularly milk kefir, show promise as low-cost, eco-friendly biosorbents, though further material modification is needed to enhance their suitability for large-scale water treatment applications.

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IDENTIFICATION OF IRON SPECIES IN BRAZILIAN CERAMICS USING MÖSSBAUER SPECTROMETRY

24

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The Goiabeiras region near Vitória in the state of Espírito Santo (Brazil) is famous for its traditional clay pots, called *panelas de barro*. They are made by local potters using a traditional technique that has been passed down for generations. The clay for their production is obtained from the area around Vitória. The pots are shaped by hand, often without a potter's wheel. After firing, the surface is coated with a decoction of mangrove bark, which gives them their characteristic dark brown to black color. It is this dark finish that is very typical of Goiabeiras ceramics. In many households, *panelas de barro* are used to serve regional dishes. They are often only sized for one serving and are served directly at the table. Such small pots are often called *panelinha de barro* (literally "little clay pot") in Brazil. Clay pots are valued because they retain heat for a very long time.

The dyeing of clay pots is one of the most fascinating and famous examples of the use of mangrove bark in the world. This process is at the heart of a centuries-old tradition that is still carried out today by indigenous artisans in the Brazilian state of Espírito Santo. Their craft has even been recognized as a national intangible cultural heritage of Brazil.

After the clay pots are pulled directly from the open fire, an extract of mangrove bark, which contains tannin, is applied while still hot. The initially reddish color of the heated pot changes to its typical, shiny, jet-black color when it comes into contact with the cold tannin liquid. This is due to a reaction with iron oxides that are naturally present in the local clay. In addition, the tannins are sealed in the pores of the clay by the heat and form a protective film. This makes the pot impermeable to water. It becomes completely smooth and ready to cook without the need for chemical glazes that could be toxic.

In this study, we used Mössbauer spectrometry to identify the iron species present in the clay from which the *panelinha de barro* is made. We also investigated their content on the surface of the pot, which was treated with a mangrove bark impregnation layer. The corresponding Mössbauer spectra clearly show the presence of iron oxides on the surface of the bowl, while they are absent in the bulk of the container material.

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SPECIATION ANALYSIS OF CHROMIUM IN PM_{10} FRACTION OF URBAN AEROSOL

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The poster deals with the seasonal and spatial variability of total chromium and its species (Cr^{3+} and Cr^{6+}) in PM_{10} fraction of particulate matter in Brno city.
The results show that the total concentration of chromium (determined in mineralized samples via ICP-MS/MS) in the air is strongly dependent on the specific location, with the highest values measured at busy intersection, confirming the significant influence of traffic.
The speciation analysis of chromium in sample extracts was performed using the HPLC-ICP-MS/MS method with isotopically enriched standards, which provided deeper insight into the stability and transformation of chromium during sample processing. The soluble (bioavailable) fraction of chromium accounted for only 15.4 ± 17.1% of the total amount. Trivalent chromium, Cr^{3+}, dominated in this soluble fraction (94.7 ± 7.7 %).
The concentration of carcinogenic hexavalent chromium (Cr^{6+}) increased during the winter sampling campaign, particularly in the area near heating plants, suggesting that transportation during the heating season represents rather a minor source of this species.
The study also identified the influence of meteorological conditions: Higher concentrations of ground-level ozone contributed to the Cr^{3+} oxidation to Cr^{6+}, while rising temperature, air pressure, global radiation and related sunshine correlated with an increase in the proportion of Cr^{3+}.

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LEACHING OF GERMANIUM SPECIES FROM SILICONE-BASED MATERIALS STUDIED BY HG-CT-ICP-MS/MS

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Germanium (Ge) is a technology-critical element used in electronics, fiber optics, infrared optics, and catalysts. In natural waters, it occurs as inorganic germanium (iGe) at ng L^{-1} levels and as methylated species such as monomethylgermanium (MMGe) and dimethylgermanium (DMGe). While iGe sources and behavior are relatively well understood, the origin and environmental dynamics of methylated species remain poorly described [1].
Due to chemical similarity between Ge and Si, we investigated silicone-based products (glues, greases, and oils) as potential sources of methylated Ge species. Polypropylene tubes were coated with each material, allowing them to cure or dry. The tubes were then filled with sub-boiled distilled water, followed by a 10-day extraction period under agitation. Total Ge and speciation were analyzed by Hydride Generation–Cryotrapping–ICP-MS/MS as described by García-Figueroa et al. [2], including an extension for trimethylgermanium (TMGe).
Total Ge in extracts ranged from below detection to 4.0 ng L^{-1} for silicone oils and 2.2 ng L^{-1} for glues. Speciation showed iGe (0.08–1.23 ng L^{-1}), MMGe (0.007–0.032 ng L^{-1}), and DMGe (0.013–0.176 ng L^{-1}). TMGe was also detected, in some cases as the dominant species (up to 5,3 ng L^{-1}), along with two unidentified Ge compounds, indicating release of more complex organogermanium species. These results suggest silicone-based materials are a potential source of methylated Ge species.

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FTIR SPECTROSCOPY FOR THE DISCRIMINATION OF SOILS WITH SIMILAR VISUAL APPEARANCE

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Soils are complex and heterogeneous materials whose composition can vary considerably despite exhibiting similar visual characteristics. Fourier transform infrared (FTIR) spectroscopy offers a rapid, non-destructive approach for probing both organic and inorganic components through their characteristic vibrational signatures. In this study, FTIR spectroscopy was used to compare two Chernozem soils of nearly identical visual appearance and colour collected from locations approximately 170 km apart. Although visually indistinguishable, the soils exhibited clear differences in their infrared spectra. Variations were observed in the O–H stretching region associated with clay minerals, in bands attributed to aliphatic organic compounds, and particularly in the intensity of characteristic carbonate absorptions. Additional differences were evident within the fingerprint region, reflecting variations in soil composition. To support interpretation of the spectral features, complementary analyses by X-ray powder diffraction (XRPD) and thermal analysis (TGA/DTG/DTA) were performed. The results demonstrate that FTIR spectroscopy is capable of revealing subtle compositional differences between visually similar soils and represents a valuable tool for rapid soil characterization.

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MAGNETO-PLASMONIC NANOCOMPOSITES AS SELECTIVE AND SENSITIVE SENSORS FOR WATER REMEDIATION

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Water monitoring is an important instrument for preventing pollution and, consequently, protecting both public health and the environment. Surface-enhanced Raman scattering (SERS), a highly sensitive analytical technique capable of detecting trace concentrations of analytes, is a promising tool for pollutant detection [1, 2]. Nanocomposites consisting of plasmonic and magnetic nanoparticles (NPs) can serve as SERS substrate owing to the optical properties of plasmonic NPs while also facilitating target extraction from the water using a simple magnetic field [2, 3]. We present magnetic NPs decorated with Au NPs via chitosan, synthesized by an environmentally friendly method. To validate SERS detection, highly charged porphyrins were chosen as model molecules. Subsequently, phenylboronic acid (PBA) was attached to the nanocomposites surface to improve selectivity, followed by SERS detection of selected pollutants containing diols (e.g. amikacin). PBA has a unique ability to reversibly bind diol-containing molecules depending on the solution pH [4]. Therefore, such functionalized magneto-plasmonic nanocomposites can be repeatedly used for the purposes of SERS detection and selective removal of pollutants from water.

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FE-BSA-AU AND MN-BSA-AU BIMETALLIC NANOCOMPOSITES FOR MAGNETIC RESONANCE AND FLUORESCENCE IMAGING

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To accurately characterize complex biological systems in the context of diseases such as cancer, neurodegenerative, and cardiovascular disorders, multimodal imaging is required. For these conditions, the combination of magnetic resonance imaging (MRI) and fluorescence imaging (FI) is widely used because of their complementary strength. MRI allows non-invasive, non-ionizing deep-tissue visualization with excellent anatomical and soft-tissue contrast, while FI offers high sensitivity and high spatial resolution at the cellular and molecular levels. For this purpose, nanocomposites combining iron oxide nanoparticles and gadolinium ions or manganese ions (providing MRI contrast) with metal nanoclusters, fluorescent dyes, or quantum dots (providing FI contrast) have been employed. Herein, we developed nanocomposites stabilized with bovine serum albumin (BSA), composed either of iron oxide nanoparticles and gold nanoclusters (Fe-BSA-Au system) [1], or of manganese ions/nanostructures and gold nanoclusters (Mn-BSA-Au system). Typical synthetic procedure consists of mixing the following precursors: $FeCl_3 \cdot 6H_2O$ or $MnCl_2 \cdot 4H_2O$, BSA as a stabilizing and reducing agent, $HAuCl_4 \cdot 3H_2O$, and finally NaOH to increase the pH of the mixture, thereby promoting the formation of nanostructures. After the addition of the final precursor, the sample is incubated at 50 °C and then purified by dialysis. The functionality of the resulting nanocomposites as bimodal imaging contrast agents was evaluated with *in vitro* MRI and FI (and *in vivo* for the Fe-BSA-Au system). Cytotoxicity was assessed prior to the *in vivo* experiments. Both imaging techniques demonstrated the potential of both systems for use as *in vitro* bimodal MRI (T_2-weighted)/FI contrast agent (additionally, in the case of Fe-BSA-Au system, even *in vivo*). Both systems were found to be non-cytotoxic toward healthy cell lines. Further research focuses on targeted cellular uptake, particularly in the islets of Langerhans.

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STEREOCHEMICAL ANALYSIS OF P-CHIROGENIC COMPOUNDS USING CHIROPTICAL SPECTROSCOPIES AND QUANTUM-CHEMICAL CALCULATIONS

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Phosphorus is an important element in both nature and modern organic chemistry. However, stereochemical analysis of P-containing compounds can be sometime rather challenging. It has been already shown that molecules with a stereogenic center on the phosphorus atom (P-chirogenic compounds) can be advantageously studied by the advanced methods of nuclear magnetic resonance (NMR) [1]. Here we demonstrate that the stereochemical information provided by NMR can be significantly enhanced through the application of chiroptical spectroscopy (electronic and vibrational circular dichroism and Raman Optical Activity). We employed rigid model molecules – phosphorylated derivatives of isopinocampheol. The experimental results were systematically correlated with *ab initio* quantum-chemical calculations [2].

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TAILOR-MADE GLASS REFERENCE MATERIALS FOR LA-ICP-MS ANALYSIS OF LITHIUM- AND URANIUM-RICH MINERALS

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Laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) is widely used for *in situ* elemental and isotopic analysis of geological materials. However, accurate quantification remains challenging when suitable matrix-matched reference materials are unavailable. This limitation is particularly important for lithium- and uranium-bearing minerals, because commonly used reference materials, such as NIST SRM series, differ substantially from these minerals in analyte concentrations, and therefore ablation behavior.

To address this issue, new silicate glass reference materials were developed for LA-ICP-MS analysis of mineral systems. Two compositional series were prepared: Li-rich glasses intended for the analysis of petalite, spodumene, and Li-rich micas, and U/Pb-rich glasses designed for studies of uranium-bearing minerals. Composition of the materials was characterized using LA-ICP-MS, micro-XRF and ICP-OES, while microscale homogeneity was evaluated by LA-ICP-MS spot analyses, elemental mapping and complementary micro-XRF measurements. Pb isotope ratios in the U/Pb-rich glasses were additionally assessed by SIMS to evaluate their potential for future geochronological applications.

Experiments revealed distinct laser-material interactions compared with conventional reference glasses. Differences in crater morphology indicate that analyte concentration plays an important role in laser ablation behavior and may influence quantitative performance.

The developed glass reference materials represent a promising tool for improving calibration strategies in LA-ICP-MS and other *in situ* analytical techniques applied to strategic raw materials.

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SERS-ACTIVE GOLD NANOPARTICLES FORMED BY SELECTED AMINO ACIDS - EFFECT OF TEMPERATURE

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Gold nanoparticles (AuNPs) exhibit unique optical and electronic properties, which can be utilised in a wide variety of applications, from electronics to biomedicine. Changes in precursor concentrations or ligand composition used for nanoparticle synthesis can tune size, shape, surface chemistry and charge of the resulting nanostructures. Chemical synthesis of nanoparticles often relies on the use of toxic chemicals as reducing and stabilising agents. On the contrary, green synthesis is a chemical method that uses safe and usually cheap chemicals, which is preferred due to increased demand for sustainability and environmental friendliness, especially in the field of nanomaterials bio-applications. It is well-known that amino acids (AA) can play the key role as both, reducing and stabilising agents in AuNPs formation; moreover, they are biocompatible and biodegradable. Synthetic parameters can be still optimized - for instance: concentrations varied, mutual molar ratios of reactants changed, physico-chemical conditions of the synthesis adjusted – e.g. temperature. The last factor has been rarely investigated so far to our best knowledge. The applicability of such AuNPs (prepared by selected AA) in surface-enhanced Raman scattering (SERS) spectroscopy is also very scarcely reported. Therefore, in this work we synthesised AuNPs owing to four different aromatic and/or hetero-aromatic AA (Tyr, Trp, Phe. and His) at different temperatures. AuNPs were then characterised by means of UV-Vis absorption spectroscopy, DLS (dynamic light scattering), ELS (electrophoretic light scattering), TEM (transmission electron microscopy) and FT-IR (Fourier-transform infrared absorption spectroscopy). The as-prepared AuNPs possessed LSPR (localized surface plasmon resonance) peak located at ~520 – 540 nm and manifested themselves by sizes of 10 – 30 nm in diameter (as verified by TEM imaging). The SERS-activity of AuNPs was investigated using model molecule TMPyP (5,10,15,20-Tetrakis(1-methylpyridinium-4-yl)porphyrin tetra(p-toluenesulfonate) and 785 nm excitation laser line. The SERS-activity was confirmed for Trp@AuNPs, Phe@AuNPs, and His@AuNPs.

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SAMPLE HOLDER FOR ANALYSIS OF LIQUIDS BY LA-ICP-MS

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In recent years, LA-ICP-MS has demonstrated significant potential for the analysis of liquid samples due to its low sample consumption and minimal impact on plasma conditions, particularly for samples with complex matrices that are immiscible with water or have high organic content, such as oils, petroleum fractions, and cosmetic products.
In our previous studies[1, 2], we addressed key challenges associated with LA-ICP-MS analysis of liquids, including sample evaporation prior to ablation and optimization of key parameters such as laser fluence, repetition rate, number of shots and droplet volume. It was demonstrated that reliable analysis on flat substrates is limited to liquids with saturated vapor pressures below approximately 60 Pa and that LA-ICP-MS results are comparable to those obtained by conventional ICP-MS using microwave-assisted acid digestion.
Although LA-ICP-MS analysis of liquid samples on flat surfaces provides satisfactory results, the use of a dedicated sample holder can significantly improve overall method robustness and repeatability. Therefore, the aim of this study was to develop a straightforward sample holder that reduces evaporation, simplifies sample handling, maximizes sample capacity, prevents sample cross-contamination and enhances analytical sensitivity.
A holder containing a series of cavities with different dimensions was fabricated and evaluated with respect to evaporation behavior and signal intensity. The optimal cavity dimensions were found to be 2 mm in diameter and 3 mm in depth, accommodating up to 9.4 µL of sample while significantly reducing evaporation and increasing signal intensity. The effects of sample volume and laser focus position on the analytical signal were also investigated. The optimized holder was successfully applied to the analysis of engine oils and cosmetic products, with results comparable to those obtained by conventional ICP-MS after microwave-assisted acid digestion.

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SENSITIVE DETERMINATION OF GERMANIUM USING HYDRIDE GENERATION, MINIATURE PLASMA AND HIGH-RESOLUTION MASS SPECTROMETRY WITH ORBITRAP ANALYZER

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Chemical hydride generation (HG) is a powerful technique for producing volatile species of elements from groups 14–16, enabling efficient matrix-free sample introduction. Among hydride-forming elements, germanium is particularly difficult to atomize in heated quartz tube, diffusion flame, and dielectric barrier discharge (DBD) atomizers, limiting the performance of atomic absorption and fluorescence spectrometry. Consequently, HG coupled with inductively coupled plasma mass spectrometry remains the primary approach for ultrasensitive total Ge determination, speciation analysis, and isotope ratio analysis.

High-resolution Orbitrap mass spectrometry (HRMS), combined with direct analysis in real time (DART), has recently been applied to mechanistic studies of HG [1] and volatile species identification [2,3]. However, its application to sensitive elemental determination following HG has not yet been explored.

In this work, HG of Ge was coupled with DART-HRMS to investigate parameters affecting ion transmission, fragmentation, and detection. GeH_4 was generated by the reaction of Ge(IV) with $NaBH_4$ in TRIS buffer and ionized in DART at 200 °C using N_2 as a discharge gas. Several instrumental parameters were optimized to maximize the signal-to-noise ratio. The highest responses were obtained in negative ion mode for $[GeO_x(H_y)]^-$ ions (x = 2–4, y = 0–3). Collision-induced dissociation approaches simplified the spectra, with GeO_2^- becoming the dominant ion. Optimization of acquisition parameters further improved sensitivity, with preliminary tests indicating a detection limit approaching the ng/l level.

The current work focuses on the development of a laboratory-made DBD ionization source to improve both ionization efficiency and analytical robustness. Two DBD designs - a tubular plasma jet and a cylindrical capillary plasma - will be presented and their analytical performance compared with that of DART.

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DISTRIBUTION OF GOLD NANOPARTICLES IN LENTIL PLANT LEAVES IMAGED BY SP-LA-ICP-MS

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Foliar application of engineered nanoparticles holds great potential for sustainable agriculture, such as nano-fertilization, yet understanding their uptake and translocation pathways requires highly precise analytical techniques. This study investigates the fate and micro-spatial distribution of gold nanoparticles (AuNPs) following foliar application on lentil (*Lens culinaris*) plants using single-particle laser ablation inductively coupled plasma mass spectrometry (SP-LA-ICP-MS). To ensure accurate particle tracking within complex plant matrices, key experimental parameters—including laser fluence, integration time, and calibration standards—were systematically optimized using matrix-matched gelatin standards. High-resolution analysis of lentil leaf cross-sections successfully resolved the localization of AuNPs. Beyond the expected surface retention, the analysis confirmed the penetration of intact AuNPs into internal leaf tissues, presumably via stomatal pathways. This internalization was followed by limited vascular translocation, with the majority of the transported nanoparticles localized in close proximity to the leaf vascular bundles. This work highlights optimized SP-LA-ICP-MS as a robust methodology for single-particle tracking in plant systems, offering critical insights into the uptake mechanisms and agronomic efficiency of foliar-applied nanomaterials.

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ABSOLUTE CONFIGURATION ASSIGNMENT OF GANAXOLONE ANALOGUES USING VIBRATIONAL CIRCULAR DICHROISM (VCD) SPECTROSCOPY AND QUANTUM-CHEMICAL CALCULATIONS

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Ganaxolone, a synthetic analogue of allopregnanolone, is a potent positive allosteric modulator of $GABA_A$ receptors and a therapeutic agent for treating epilepsy and neuropsychiatric disorders.[1] To analyze metabolic stability, pharmacokinetics and potency, a series of Ganaxolone analogues and their isomers was synthesized. Structural assignment based solely on ^{1}H and ^{13}C NMR remains challenging. Moreover, electronic circular dichroism (ECD), which is often used for steroid studies, is unsuitable here: the sole UV-vis chromophore present - a carbonyl group - is situated too distant from the stereocenters which differ in their chiral configurations. In contrast, VCD spectroscopy in combination with QM calculations enables discrimination of all studied analogs and their isomers, allowing for unambiguous determination of their stereochemistry, including absolute configuration.

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HYDROGEL-ASSISTED SERS: ALGINATE–SILVER COMPOSITE SUBSTRATES

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In recent years, hydrogels have attracted growing attention as promising substrates for surface-enhanced Raman spectroscopy (SERS) due to their unique properties and several advantages over traditional SERS platforms, such as colloidal nanoparticle dispersions or metallic nanoparticle coatings deposited on rigid supports. Their optical transparency and inherently low spectral background make hydrogels particularly suitable for Raman-based analyses. Furthermore, their highly hydrophilic and flexible structure, arising from extensive hydrogen bonding and strong water-retention capability, can effectively reduce the coffee-ring effect that frequently occurs during analyte deposition on solid surfaces. Hydrogels may also contribute to improved nanoparticle stability, with sodium alginate being especially attractive because of its favorable stabilizing properties. Consequently, alginate-based hydrogels were selected as the subject of the presented ongoing study.

The aim of this work is to develop and evaluate AgNPs–alginate hydrogel composites as SERS-active materials. Silver nanoparticles were prepared using trisodium citrate as reducing agent. Into the prepared colloidal solution sodium alginate was dissolved and the formation of the hydrogel network was achieved through ionic cross-linking with calcium ions (Ca^{2+}). The resulting composites were characterized by UV–Vis spectroscopy, Raman spectroscopy, Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM). and energy dispersive spectroscopy (EDS).

The SERS performance of the prepared substrates was examined using excitation wavelengths of 455, 633, and 785 nm. Representative Raman probe molecules, namely rhodamine B, rhodamine 6G, crystal violet, adenine and others. Analytical enhancement factors were determined, and detection limits were established for each substrate–analyte system. Signal reproducibility was assessed by calculating the relative standard deviation (RSD) from measurements acquired at ten different locations on each substrate. Additionally, the long-term stability of the hydrogels was investigated and SERS activity of the samples stored in their hydrated form with dried samples that were rehydrated in analyte solutions prior to SERS measurements compared.

MAGNETIC AND MÖSSBAUER INVESTIGATIONS OF ANIMAL LIVER TISSUE

38

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Iron is an essential bioelement key to oxygen transport and hematopoiesis, with the liver serving as its primary storage organ. In the mammalian liver, approximately 80% of iron in hepatocytes is bound by ferritin, around 2–3% is present as heme, and the remainder exists as transferrin-bound iron or within the labile intracellular pool. Structurally, ferritin encapsulates this iron within its protein shell as a hydrous ferric oxide nanoparticle closely resembling ferrihydrite FeOOH.

We have investigated the spin transition from the paramagnetic state at low temperatures to the diamagnetic state by increasing the temperature using magnetic measurements and Mössbauer spectroscopy. The field dependence of magnetic moment in the temperature range 2K - ~ 20 K corresponds to paramagnetic state with Low Spin (LS) electron configuration of $Fe2^{+}$ S=0, $t_{2g}{}^{6}e_{g}{}^{0}$. By increasing temperature, transitions to the diamagnetic state with electron configuration in High Spin (HS) S=2, $t_{2g}{}^{4}e_{g}{}^{2}$ occur. The magnetic state between 20 K to 40 K can be interpreted as mix of paramagnetic and diamagnetic states, i.e. gradual change from LS to HS.

ENVIRONMENTAL STRESS AND CHEMICAL STABILITY IN FORENSIC EVIDENCE: A VIBRATIONAL SPECTROSCOPY STUDY

39

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Modern forensic science increasingly prioritizes tracking the chemical maturation of forensic evidence under fluctuating environmental stresses. In this context, vibrational spectroscopy is investigated as a promising, non-invasive technique to capture such dynamic shifts with minimal sample handling.

Our project utilizes a bespoke environmental chamber to simulate specific conditions (temperature, humidity) and monitor temporal spectral variations in both model and authentic biological fluids (blood, saliva) across different surfaces. The degradation pathways are significantly modulated by environmental parameters and substrate interactions, with the expectation that distinct spectral markers could serve as indicators for estimating the post-deposition interval of biological traces.

Building on this framework, we extend our methodology to the trace detection of exogenous substances, particularly drugs and metabolites, within saliva. By employing surface-enhanced vibrational techniques, we achieve sensitive identification while addressing challenges posed by biological variability and spectral overlap [1].

Furthermore, we apply these stability principles to synthetic matrices, specifically analyzing the compositional diversity and thermal resilience of electronic cigarette liquids (e-liquids). By employing flow-through ATR infrared spectroscopy, we aim to observe real-time aerosol generation and track temperature-driven spectral shifts that reflect the thermal degradation of components.

Our research demonstrates that vibrational spectroscopy can effectively map chemical evolution, potentially offering robust solutions for determination of “time since deposition”, trace contaminant screening, and aerosol characterization.

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Acknowledgements

This work was supported by the grant of Specific university research – project „*Dynamics of Forensic Samples - Their Controlled Ageing Using Vibrational Spectroscopy Optics*”.

SERS DETECTION OF ATROPINE IN *DATURA* AND *BRUGMANSIA*: FROM RAW MATERIAL TO OPTIMIZED EXTRACTION

40

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The *Datura* and *Brugmansia* species are notoriously known for containing highly toxic tropane alkaloids posing significant risks when these plants contaminate food crops. Moreover, as they are frequently cultivated in gardens, they present a direct hazard to children and pets, with toxic atropine present in all plant parts - from blossoms and leaves to roots and seeds. Direct vibrational spectroscopic analysis of raw plant material is challenging due to complex matrices rich in primary metabolites (in infrared spectra, fig. 1), strong fluorescence interference (in Raman spectra), and insufficient sensitivity for trace detection of atropine.

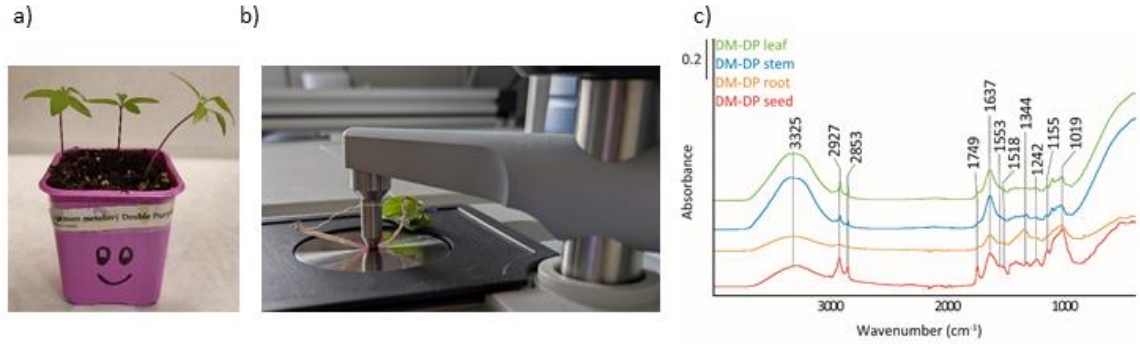

Fig. 1: a) cultivated plants of *Datura metel*, b) measurement of infrared spectra of raw plant material, c) comparison of infrared spectra of *Datura metel* different parts

To overcome these challenges, this study aimed to develop a robust Surface-Enhanced Raman Scattering (SERS) procedure for the successful detection of atropine through optimized sample preparation and instrumental parameters. We conducted a comprehensive comparative analysis of raw materials versus extracts. Our approach involved systematically evaluating spectral features, identifying that while raw spectra were saturated with lipids, polysaccharides, and proteins, the extraction process successfully isolated soluble secondary metabolites, including phenolic compounds such as alkaloids and flavonoids. The extracts were analyzed using optimized silver nanostructured substrates, prepared from aggregated colloidal silver systems and dried on aluminum foil. SERS analysis of the extracts confirmed the presence of atropine in *Datura* and *Brugmansia* species at concentrations reaching 10^{-7} mol/L.

IRON REDOX AND STRUCTURAL CHANGES IN FUNGAL-MEDIATED MAGNETITE ALTERATION REVEALED BY SPECTROSCOPY

41

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Metabolically active filamentous fungi naturally possess a high capacity to alter the physicochemical composition of nearby minerals. This is typically initiated and facilitated by acidolysis, a process involving the secretion of acidic or redox active compounds that promote mineral dissolution, extracting metallic ions into the extracellular environment. The biochemically induced extraction of elements from solid (mineral) phases is commonly known as bioleaching, which, besides chemical interactions, also involves physical interplay between microbial cells and solid mineral surfaces. These naturally occurring processes affect the mineralogy of iron oxides, e.g., magnetite, in the vicinity of growing microorganisms to various extents. Thus, in our study, we have addressed the critical issue of fungal impact on the structural and chemical stability of magnetite using Mössbauer spectroscopy and other techniques suitable for solid phase and elemental analysis. Our outcomes provide insights into the mineralogical and structural alterations induced by fungal interactions with magnetite nanopowder. While *A. clavatus* showcased the ability to trigger crystal lattice distortions in magnetite, suggesting its potential to induce structural changes even with limited bioleaching activity, *A. niger* strain exhibited minimal impact on the structural properties and mineralogy of magnetite during cultivation, highlighting magnetite mineralogical stability even under acidic conditions.

Acknowledgements
This work was supported by the Scientific Grant Agency of the Slovak Republic Ministry of Education and the Slovak Academy of Sciences under VEGA contract No. 1/0484/26. It was also supported by the Slovak Spectroscopic Society, member of the Association of Slovak Scientific and Technological Societies with the following logo:

CU NANOCLUSTER-EMBEDDED PVDF ELECTROSPUN FIBERS: VIBRATIONAL, OPTICAL AND ELECTRICAL CHARACTERIZATION

42

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Poly(vinylidene fluoride) (PVDF) is an important electroactive polymer widely used in flexible sensors, nanogenerators and multifunctional devices due to its chemical stability, processability and piezoelectric β-phase [1]. In this work, Cu nanocluster-containing PVDF electrospun fibers were prepared to develop multifunctional fibrous mats with combined optical and electrical responses. Cu nanoclusters were synthesized in N,N-dimethylformamide and incorporated into PVDF electrospinning solutions under different Cu content and co-solvent ratios. The prepared Cu/PVDF electrospun mats were characterized using vibrational spectroscopy, optical spectroscopy, microscopy and electrical measurements. Fourier-transform infrared spectroscopy was used to analyse the characteristic vibrational bands of PVDF and to evaluate the relative β-phase fraction in pristine PVDF and Cu/PVDF fibers. The results showed that stable fiber formation played an important role in maintaining the electroactive β-phase. Cu incorporation modified the fiber morphology and electrical response; however, in well-formed fibers, the β-phase fraction remained relatively comparable to pristine PVDF. Optical absorption and fluorescence measurements confirmed the optical response of the Cu-containing dispersion, indicating its potential contribution to fluorescence functionality in the composite fibers. Dielectric measurements showed an enhanced polarization response after Cu incorporation, which was mainly attributed to Cu/PVDF interfacial polarization and morphology-dependent charge distribution rather than only to β-phase enhancement. Therefore, this study demonstrates that Cu nanocluster incorporation can modify the functional behaviour of PVDF electrospun fibers while preserving their electroactive character. The combination of vibrational spectroscopy with optical and electrical characterization provides useful insight into the structure–property relationship of Cu/PVDF fibrous materials for potential sensing and energy-harvesting applications.

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Acknowledgements

Financial support by the Internal grant agency of Palacký University (project no. IGA_PrF_2026_017) is gratefully acknowledged.

DITHIOTHREITOL INDUCING GOLD NANOSTRUCTURES FORMATION

43

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Gold nanostructures (AuNSs) possess unique optical properties. When preparing them from individual atoms (i.e. by bottom-up synthetic pathway), one can generate either nanoclusters or nanoparticles based on the conditions of synthesis. While Au nanoclusters (AuNCs) can reveal luminescence in the visible region of electromagnetic radiation; Au nanoparticles (AuNPs) are well-known for their surface plasmon resonance band positioned also in the visible region that is convenient for AuNPs application, namely in surface-enhancement of optical phenomena – e.g. Raman scattering.
The aim of the present work is to investigate the role of dithiothreitol (DTT) in AuNSs preparation. It is known from the literature [1] that DTT can be used as both, reducing and stabilizing agent when interacting with Au (III) precursor. Therefore, in the present study, we focused on the selected five molar ratios of Au (III) : DTT (1:3, 1:2, 1:1, 2:1, and 3:1) under four relevant pH values (7, 8, 9, 10). Several spectroscopic and microscopic methods available in our labs were used for AuNSs characterization, such as: UV-Vis spectroscopy, dynamic light scattering, zeta potential measurements, steady-state fluorescence spectroscopy, Raman spectroscopy, infrared absorption spectroscopy, and transmission electron microscopy. From the results, it can be stated that the molar ratios of 1:3 and 1:2 of Au (III): DTT resulted in AuNCs formation, whereas the excess of Au (III) led to AuNPs generation. Both types of AuNSs were obtained in pH values varied between 8-10. Molar ratio of 1:1 of Au (III): DTT led most probably to the complexation of Au (III) with DTT since no AuNCs, nor AuNPs formation was observed. The successfully formed AuNPs served as efficient surface-enhanced Raman scattering substrates for a selected model adsorbate (anionic porphyrin) detection in 0.1 μM final concentration. It is envisaged that this type of AuNPs synthesis could be further exploited in magneto-plasmonic nanocomposite generation.

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Acknowledgements

Financial support by the Czech Science Foundation (project no. 25-15590S) is gratefully acknowledged. The authors also acknowledge IGA_PrF_2026_017.

DETERMINATION OF SOIL PARAMETERS, AND Fe, Mn, Al CONTENT USING THE F-AAS

44

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Iodine is an essential element for humans, playing a crucial role in the production of thyroid hormones. Its bioavailability in soil is strongly influenced by soil physicochemical properties, which control its mobility and retention. In addition, soil microorganisms, particularly microscopic filamentous fungi, may affect iodine availability through the production of extracellular metabolites that modify soil chemical conditions and promote iodine mobilization. The aim of this study was to determine selected soil parameters of cultivated Fluvisol and cultivated Chernozem with emphasis on their potential influence on iodine behavior in soil. Therefore, soil pH, total organic carbon (TOC), total Fe, Mn, and Al contents, as well as their amorphous fractions, were determined using Flame Atomic Absorption Spectrometry (F-AAS). These parameters were selected due to their key role in iodine sorption and bioavailability.
The results showed clear differences between the studied soils, with Chernozem exhibiting a higher potential for iodine retention due to its higher organic matter content and greater abundance of amorphous Fe and Al phases. This creates stronger sorption capacity for iodine and more suitable conditions for studying its release mechanisms.
Based on the results obtained, cultivated Chernozem was identified as a more suitable substrate for subsequent biofortification experiments and for investigating the mobilization potential of fungal metabolites. Overall, Chernozem provides a better model system for studying interactions between iodine, soil components, and microbial metabolites, as well as for evaluating microbially assisted iodine biofortification in plants.

Acknowledgements
This work was financed by the EU Next Generation EU through the Recovery and Resilience Plan of the Slovak Republic under Project No. 09I03-03-V04-00123 and by the Slovak Spectroscopic Society, a member of the Association of Slovak Scientific and Technical Societies, whose logo is displayed below

DEVELOPMENT OF (LA)-ICP-MS ANALYTICAL METHODOLOGY FOR ELEMENTAL ANALYSIS OF HISTORICAL SILVER COINS AND ASSESSMENT OF ISOTOPE ANALYSIS POSSIBILITIES

45

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Building upon previous research on the chemical analysis of historical silver coins, the presented work focuses on the development and optimization of advanced analytical methodologies based on ICP-MS, including laser ablation (LA-ICP-MS). Particular emphasis is placed on improving the accuracy and precision of elemental analysis through the preparation and validation of in-house matrix-matched reference materials. These standards closely resemble the complex composition of historical silver alloys, thereby reducing matrix effects and improving data reliability.
In parallel, solution-based ICP-MS is utilized to assess the potential of lead isotope analysis for determining the geographical origin of the silver ore. To support this liquid-sample approach, electrogravimetric separation of the silver matrix is being optimized. This process is crucial for preventing silver deposition within the instrument interface, thereby ensuring the stability required for isotopic measurements.
By combining elemental fingerprinting with the preliminary assessment of isotopic ratios, this research aims to provide a more reliable interpretation of compositional data and contributes to the understanding of metallurgical practices and raw material sourcing in historical coinage. The proposed methodologies are critically evaluated with respect to their applicability in micro-destructive and non-destructive archaeological research.

Acknowledgments
This research was supported by the Grant Agency of Masaryk University project no. MUNI/C/0129/2026

A PRACTICAL HR-CS ET-AAS METHOD FOR PHOSPHORUS DETERMINATION IN PLANTS AND FOODS

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Accurate quantification of phosphorus in plants and foods is essential for both nutritional evaluation and agricultural assessment. This contribution presents a straightforward and highly practical HR-CS ET-AAS method for total phosphorus determination using atomic absorption at 213.618 nm.
Under optimized conditions (atomization at 2700 °C) with an excess of Pd/Mg(NO_3)$_2$ modifier, spectral interferences from molecular phosphorus monoxide (PO) are effectively suppressed. The method achieves a detection limit of 0.2 mg/L and a wide calibration range up to 80 mg/L. This approach represents an advantageous alternative to other available techniques. Compared to molecular absorption spectrometry (HR-CS ET-MAS), this atomic absorption-based determination is less prone to spectral and non-spectral interferences. It also provides superior selectivity over traditional colorimetric methods. Furthermore, it is a viable alternative to ICP-MS, where phosphorus determination is hindered by severe isobaric interferences and excessive sensitivity. The working range is comparable to that of ICP-OES; however, the AAS-based approach offers lower operational costs and requires smaller sample volumes (30 µL for triplicate measurements).
The method is routinely used for the analysis of diverse matrices, including meat, bakery products, sewage sludge, insects, nuts, fruits, and vegetables.

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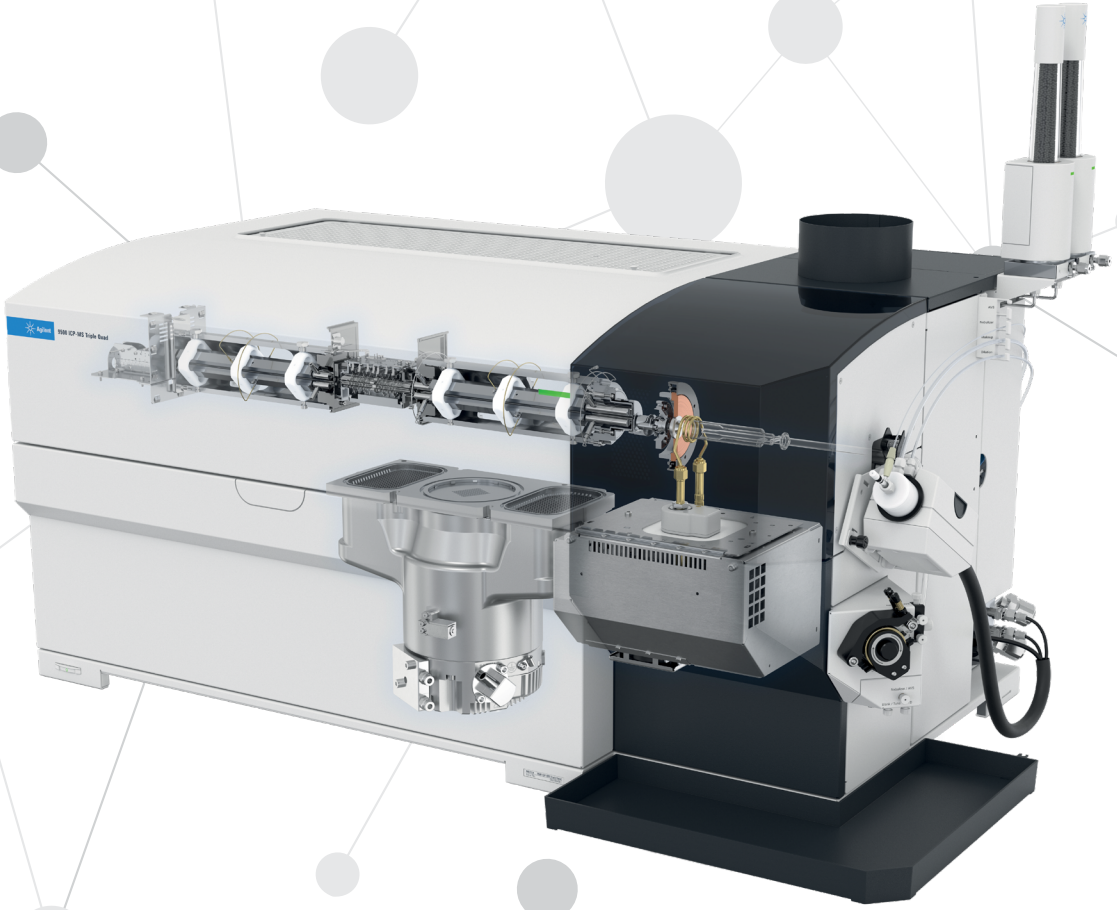

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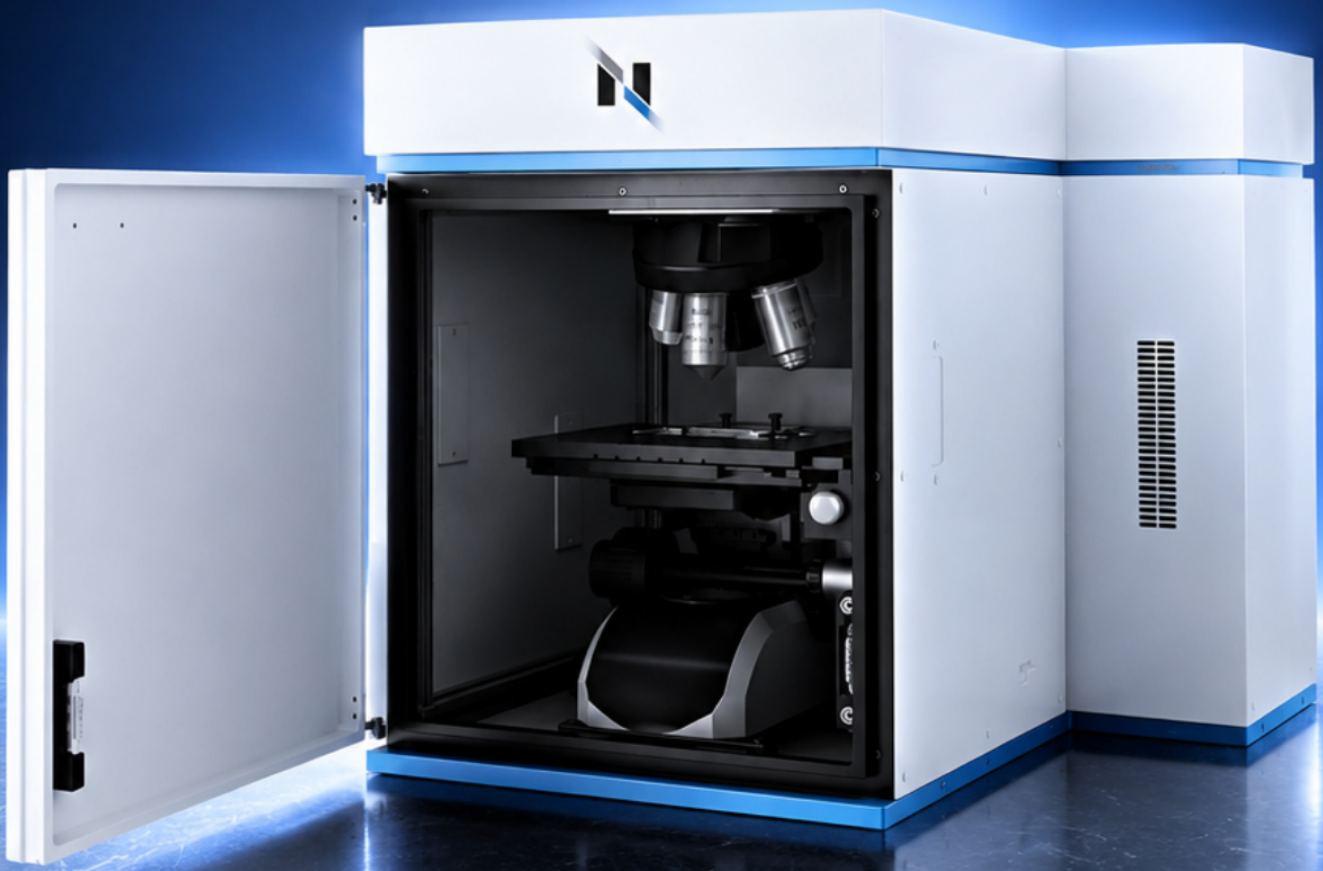

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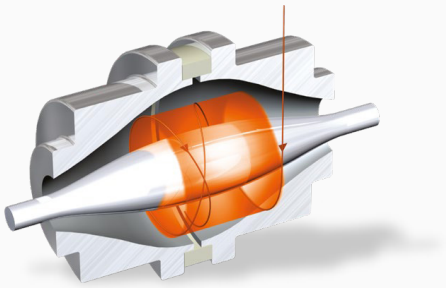

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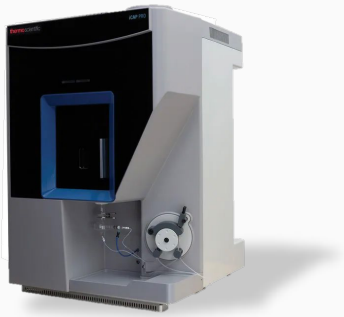

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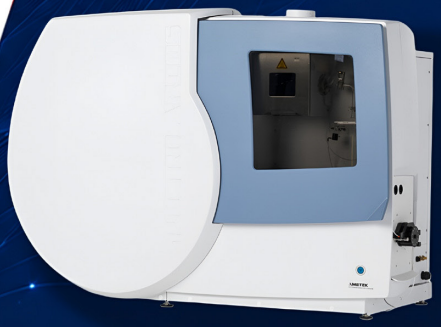

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