



Kurdějov
2024



Mössbauer Spectroscopy
in Materials Science 2024

BOOK OF ABSTRACTS

MAY 27–31, 2024

MUNI
SCI



Palacký University
Olomouc



UNIVERSITY OF
CHEMISTRY AND TECHNOLOGY
PRAGUE



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The 18th Czech-Slovak Spectroscopic Conference (18th CSSC) is the 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 as well as look into future development. The aim of this scientific event is **to bring together experts** from universities, academia, official centers, 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.

The microsposium entitled "**Recent progress in vibrational spectroscopy - Celebrating 50 years of SERS and the 65th anniversary of A. Smekal death**" is the inherent part of the Conference programme as a parallel session. Invited as well as short lectures in the Microsymposium will cover a wide range of topics targeted on recent progress in Raman and infrared spectroscopy and their applications. A particular attention will be given to special methods of Raman spectroscopy, namely resonance Raman scattering (RRS) and surface-enhanced/resonance/Raman scattering (SERS and SERRS) as well as to time-resolved IR and Raman spectroscopy. Moreover, the development and application of advanced techniques of vibrational spectroscopis imaging/mapping both in micro- and nanoscale will be covered. Furthermore, application of IR and Raman spectroscopy in various branches of chemistry, material science, geology, gemmology, art conservation, environmental science, food processing, biology and medicine will be an inherent part of the Microsymposium scope.

The upcoming year of this conference with a long tradition differs from the previous ones by a greater emphasis on analytical spectrometry applied in **the geological sciences**. Many scientists with a geological background are engaged in laboratory analysis and research of geological materials. These geologists are experts not only in their parent field, but also bring new knowledge in the methodology of analytical chemistry, namely spectrometry. Contributions to the conference program in the field of analysis of geological materials are therefore very much in demand, as well as participants - geologists, who are warmly welcome to this conference.

A series of specialized colloquia entitled "**Mössbauer Spectroscopy in Materials Science (MSMS)**" was initiated in the Central Europe. They have been almost regularly organized since 1994 alternatively in Slovakia and 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 organizers 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.

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Kamil Sobek	
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Tomáš Vašina	



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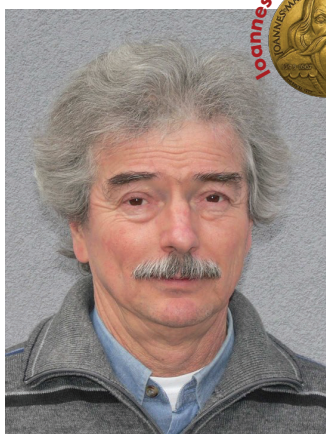
MEDALISTS

MEDAL AWARDS

Since the year of 1977, the Ioannes Marcus Marci Spectroscopic Society has been awarding the **Ioannes Marcus Marci of Kronland Medal** to distinguished individuals in the field of spectroscopy. Named after the renowned Czech scientist, physician, and academic dignitary of Charles University, this medal was first presented on the occasion of the XX Colloquium Spectroscopicum Internationale in Prague. It is awarded in recognition of local and foreign scientists for their outstanding work and contributions in any of the spectroscopic fields. In the international context, this medal is of extraordinary significance and is considered an event worthy of, among other things, reports in renowned scientific journals. Each year, a rather limited number of the medals are awarded and the nominees are selected following a very critical evaluation.

The **Nicolaus Konkoly-Thege Medal** is awarded by the Slovak Spectroscopic Society for significant contributions to the development of spectroscopy in Slovakia and throughout the world. It was first awarded in 2010 and bears the name of the extraordinary scholar and prominent, internationally recognized scientist, physicist, and astronomer, Dr. Mikuláš Konkoly-Thege. Based on his scientific merits, Dr. Konkoly-Thege became a member of several foreign scientific organizations and a recipient of various awards. However, his most significant achievements included the founding of the Hurbanovo Observatory, an astrophysical observatory still in operation today.

OUR MEDALISTS:



Prof. Ernest Beinrohr

University of St. Cyril and Methodius in Trnava, Slovakia



Prof. Ewa Bulska

University of Warsaw, Poland



Prof. Martin Hof

J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic

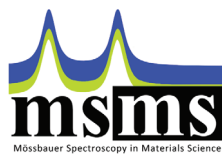


Prof. Viktor Kanický

Masaryk University, Brno, Czech Republic



PROGRAMME



Conference programme

Monday

27

May

15:00-18:00

Registration

18:00-21:00

Welcome party

Tuesday

28

May

Registration/opening 8:15-9:00

Chair: Kanický ● Beinrohr 9:00-9:45

Vyshnikin 9:45-10:15

Coffee break 10:15-11:00

CSSC lectures will be in Vinař, MSMS in Kasáda and Microsymposium in Adina



Lecture hall - Vinař

Chair: Čáslavský

11:00-11:30 Brecker

11:30-11:50 Zini

11:50-12:10 Fiala

12:10-12:30 Havránek

12:30-12:50 Mehwish

Lecture hall - Kaskáda

Chair: Machala

11:00-11:30 Greneche

11:30-11:50 Kuzmann

11:50-12:10 Dubiel

12:10-12:30 Kořenek

12:30-12:50 Košovský

Hotel restaurant

12:50-14:30 Lunch

Lecture hall - Vinař

Chair: Urík

14:30-15:00 Košek

15:00-15:20 Matoušek

15:20-15:40 Holá

15:40-16:00 Sobek

16:00-16:20 Dobeš

Lecture hall - Kaskáda

Chair: Oshtrakh

14:30-15:00 Garcia

15:00-15:20 Pechoušek

15:20-15:40 Skoumal

15:40-16:00 Vondrášek

16:30-16:50 Group photo shoot

17:00-19:00 Poster session

19:00-21:00 Dinner

Conference programme

Monday

27

May

15:00-18:00 Registration

18:00-21:00 Welcome party

Lecture hall – Vinař

Tuesday

28

May

Chair: Kanický

8:15-9:00

Registration/opening

9:00-9:45

● **Beinrohr**

Trace analysis of metals and nonmetals by line and continuum source aas coupled online with electrochemical preconcentration techniques

9:45-10:15

Vyshnikin

In-vessel headspace liquid-phase microextraction

10:15-11:00

Coffee break

Chair: Čáslavský

11:00-11:30

Brecker

Complexation between Aconitine and Various Flavonoides as Possible Concept for Detoxification: A Spectroscopic View on the Complex Formation

11:30-11:50

Zini

Timegated Raman -True fluorescence suppression

11:50-12:10

Fiala

NMR spectroscopy of nucleic acids in living mammalian cells

12:10-12:30

Havránek

Preparation and characterization of porous silver films by ion sputtering followed by ion irradiation

12:30-12:50

Mehwish

Finding conditions for Monometallic and Bimetallic Platinum-containing nanoclusters' formation

12:50-14:30

Lunch

Chair: Urík

14:30-15:00

Košek

A decad of portable Raman spectrometers in mineralogical studies

15:00-15:20

Matoušek

Nové technologie v Ramanově spektrometrii: Zobrazování pomocí liniového laseru a High Throughput Virtual Slit

15:20-15:40

Holá

LA-ICP-MS: A key to detailed imaging of trace elements in geological samples

15:40-16:00

Sobek

Spectroscopical approach for studying biological shielding concrete

16:00-16:20

Dobeš

Lead isotopic analysis: Back to basics, potential of current analytical techniques & visions for future improvements

16:30-16:50

Group photo shoot

17:00-19:00

Poster session

17:00-19:00

Dinner



Conference programme

Monday

27

May

15:00-18:00

Registration

18:00-21:00

Welcome party

Lecture hall – Kaskáda

Tuesday

28

May

11:00-11:30

Greneche

Local Structural and Magnetic properties of Fe containing nanoarchitectures

11:30-11:50

Kuzmann

Mössbauer AND XRD observation of the effect of swift heavy ion irradiation in nano-maghemite

11:50-12:10

Dubiel

Microscopic phenomena in Fe-Cr alloys

12:10-12:30

Kořenek

Structure analysis of Surface-manufactured CL20ES samples prepared by slm

12:30-12:50

Košovský

Precipitation of ODS steels after long-term annealing

12:50-14:30

Lunch

Chair: Machala

Chair: Oshtrakh

14:30-15:00

Garcia

Adsorption of some metal contaminants in water using akageneite nanoparticles: spectroscopic and kinetic studies

15:00-15:20

Pechoušek

Mössbauer, XRD and SEM/EDX spectroscopic study of DC magnetron sputtered AISI 304 stainless steel films

15:20-15:40

Skoumal

Enhancing Mössbauer Spectroscopy for Efficient Quality Control in Metallurgical Industries

15:40-16:00

Vondrášek

Fast ^{57}Fe Mössbauer austenitemeter

16:30-16:50

Group photo shoot

17:00-19:00

Poster session

17:00-19:00

Dinner



Conference programme

Wednesday

29
May

8:15-9:00	Bulska ● Chair: Kratzer
9:00-9:30	Cialla-May
9:30-10:00	Deckert
10:00-10:45	Coffee break

Lecture hall - Vinař

Chair: Kaňa

10:45-11:15	Musil
11:15-11:35	Hájková
11:35-11:55	Cyprichová
11:55-12:15	Kratzer
12:15-12:35	Figueroa

Lecture hall - Adina

Chair: Cialla-May

10:45-11:15	Procházka
11:15-11:45	Dendisová
11:45-12:15	Vlčková
12:15-12:35	Palounek

Lecture hall - Kaskáda

Chair: Schünemann

10:45-11:15	Dubiel
11:15-11:35	Yaroslavtsev
11:35-11:55	Kubuki
11:55-12:15	Grey
12:15-12:35	Klencsár

Hotel restaurant

12:35-14:00 Lunch

Lecture hall - Vinař

Chair: Holá

14:00-14:30	Limbeck
14:30-14:50	Marek
14:50-15:10	Hrdlička
15:10-15:30	Bosáková
15:30-15:50	Krempf
15:50-16:30	Coffee break

Chair: Šebesta

16:30-17:00	Kaňa
17:00-17:20	Zvěřina
17:20-17:40	Matoušek

Lecture hall - Adina

Chair: Lendl

14:00-14:30	Kloz
14:30-15:00	Šišková
15:00-15:30	Kočišová
15:30-16:00	Mojzeš

Chair: Deckert

16:30-17:00	Kalbáčová
17:00-17:30	Němec
17:30-18:00	Kalbáč

Lecture hall - Kaskáda

Chair: Homonnay

14:00-14:30	Barrero
14:30-14:50	Goneková
14:50-15:10	Lančok
15:10-15:30	Oshtrakh
15:30-15:50	Németh

Chair: Dubiel

16:30-17:00	Homonnay
17:00-17:20	Procházka
17:20-17:40	Heger
17:40-18:00	Koutný
18:00-18:20	Lisníková

19:30-?? Conference dinner

Conference programme

Lecture hall – Vinař

Wednesday

29

May

8:15-9:00

● **Bulska**

Chair: Kratzer

From Isotope Fractionation to Chemical Speciation of Biologically Relevant Substances

9:00-9:30

Cialla-May

Surface enhanced Raman spectroscopy in bioanalytics

9:30-10:00

Deckert

Tip-Enhanced Raman Scattering - old stories and new developments

10:00-10:45

Coffee break

Chair: Kaňa

10:45-11:15

Musil

Recent advances in photochemical vapor generation of several technology-critical elements

11:15-11:35

Hájková

Analytika s.r.o., Czech manufacturer of ref. materials for labs

11:35-11:55

Cyprichová

Application of six-step sequential extraction for determination of zinc fractions in paddy soils

11:55-12:15

Kratzer

Laser induced fluorescence: A reliable tool for diagnostics and development of hydride atomizers

12:15-12:35

Figueroa

Plasma assisted vapor generation of platinum group elements

12:35-14:00

Lunch

Chair: Holá

14:00-14:30

Limbeck

Spatially resolved material analysis using a combined LA-ICP-MS and LIBS procedure

14:30-14:50

Marek

Analysis of metals by atomic spectrometry

14:50-15:10

Hrdlička

Laser-induced breakdown spectroscopy in analysis of algae

15:10-15:30

Bosáková

Acoustic/optical emission spectroscopic hyphenated data from laser-induced plasmas. From the concept to the scene

15:30-15:50

Krempl

Imaging of uranium ores by laser induced breakdown spectroscopy (LIBS)

15:50-16:30

Coffee break

Chair: Šebesta

16:30-17:00

Kaňa

Exploring the environmental role of arsenic speciation in macrofungi

17:20-17:40

Zvěřina

Simultaneous determination of Pb, Al, and Fe in the analysis of Antarctic terrestrial flora using HR-CS GF-AAS

17:40-18:00

Matoušek

Speciation of Arsenic, antimony, Germanium and Tellurium in drinking water reservoirs over the seasons of the year

19:30-??

Conference dinner



Conference programme

Lecture hall – Kaskáda

Wednesday

29

May

Chair: Schünemann

10:45-11:15	Dubiel	Mössbauer spectroscopic insight into effect of magnetism on lattice vibrations
11:15-11:35	Yaroslavtsev	New nuclear resonance beamline ID14 at ESRF
11:35-11:55	Kubukl	Development of tin oxide particles distributed phosphovanadate glass as a cathode for secondary battery with high performances
11:55-12:15	Grey	^{119}Sn Mössbauer spectrometry used in the study of Tin-containing metallic glasses
12:15-12:35	Klencsár	Mössbauer study of Platinum-decorated iron oxide powders developed for gas sensing applications

12:35-14:00 Lunch

Chair: Homonnay

14:00-14:30	Barrero	Mössbauer Studies of β -Hematin Crystals: Bridging Gaps in Malaria Research
14:30-14:50	Goneková	Mössbauer Spectroscopy Analysis of Fungal-Induced structural changes in Ochres
14:50-15:10	Lančok	Bio- and chemical applications of Mössbauer spectroscopy
15:10-15:30	Oshtrakh	How many iron compounds are in pharmaceuticals containing ferrous bisglycinate chelate? Study using Mössbauer spectroscopy
15:30-15:50	Németh	Is there something really new in the field of materials analysis? Spoiler: Yes, there is

15:50-16:30 Coffee break

Chair: Dubiel

16:30-17:00	Homonnay	Mössbauer analysis of the goethite and hematite content of paleosols and goethite nodules from the Carpathian basin region
17:00-17:20	Procházka	Quantitative analysis in Mössbauer spectroscopy
17:20-17:40	Heger	Electrodeposition of ^{57}Fe iron thin films on piezofilms for Mössbauer gamma optics
17:40-18:00	Koutný	Comparison of scintillation and semiconductor detectors in mössbauer spectroscopy
18:00-18:20	Lisníková	Controlling the properties of Nanosized CoFe_2O_4 Prepared with the hydrothermal synthesis

19:30-?? Conference dinner

Conference programme

Lecture hall – Adina

Wednesday

29

May

Chair: Cialla-May

10:45-11:15	Procházka	50 years of surface-enhanced raman spectroscopy: From fundamentals to innovative applications
11:15-11:45	Dendisová	Exploring the Synergy of Electrochemistry and Surface-Enhanced Raman Scattering (EC-SERS) for Advanced Surface Analysis
11:45-12:15	Vlčková	The role of adsorption sites on Ag nanoparticle surfaces in SERS spectroscopy and plasmon catalysis
12:15-12:35	Palounek	Interferometric scattering microscopy revealing hotspot dynamics during fluctuations in single molecule Raman spectroscopy
12:35-14:00	Lunch	

Chair: Lendl

14:00-14:30	Kloz	Femtosecond stimulated Raman spectroscopy in deciphering switching mechanism of biological photoreceptors
14:30-15:00	Šišková	Noble metal nanostructures used in spectroscopies
15:00-15:30	Kočišová	Droplet deposition Raman spectroscopy techniques and their applications
15:30-16:00	Mojzeš	Raman microscopy of cells and tissues: From crystalline inclusions to viral factories
16:00-16:30	Coffee break	

Chair: Deckert

16:30-17:00	Kalbáčová	Cryomagnetic spectroscopies on van der waals materials using chiral light
17:00-17:30	Němec	Combined vibrational spectroscopic and structural study of molecular NLO materials
17:30-18:00	Kalbáč	Application of Raman spectroscopy in the studies of 2D materials

19:30-?? **Conference dinner**



CZECH-SLOVAK
SPECTROSCOPIC
CONFERENCE

2024



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Mössbauer Spectroscopy
in Materials Science 2024

Conference programme

Thursday

30
May

8:30-9:15	Kanický ● Chair: Němec
9:15-9:45	Lendl
9:45-10:05	Kuižová
10:05-10:25	Kopal
10:25-11:00	Coffee break

Lecture hall - Vinař

Chair: Vaculovič

11:00-11:30	Preisler
11:30-11:50	Humplík
11:50-12:10	Biskupič
12:10-12:30	Bahelková

Lecture hall - Adina

Chair: Němec+VIčková

11:00-11:30	Profant
11:30-12:00	Kapitán
12:00-12:20	Jílek
12:20-12:30	Closing

Lecture hall - Kaskáda

Chair: Greneche

11:00-11:30	Schünemann
11:30-11:50	Jakubowska
11:50-12:10	Mašláň

Hotel restaurant

12:30-13:30 Lunch

14:00-18:30 Trips and excursions

19:00-21:00 Dinner

21:00-21:15 Ceremony awards



Conference programme

Lecture hall – Vinař

Thursday

30
May

		Chair: Němec	
8:30-9:15	● Kanický	Czech and Slovak spectroscopy interactions - history and future	
9:15-9:45	Lendl	Laser-Based MID-IR Absorption and Dispersion Spectroscopy of Liquids	
9:45-10:05	Kuižová	Thermotropic phase transition of dehydrated phospholipids monitored by drop coating deposition Raman (DCDR) spectroscopy	
10:05-10:25	Kopal	Exploring Conformational Changes via Surface-Enhanced Raman Spectroscopy Assisted by Interferometric Scattering Microscopy	
10:25-11:00	Coffee break		
		Chair: Vaculovič	
11:00-11:30	Preisler	Nanoparticle Counting by Laser-Assisted Mass Spectrometry	
11:30-11:50	Humplík	Arsen, selen, titan.... singlequadem se nedoměřiš	
11:50-12:10	Biskupič	Nanoparticles as a new tool to diagnose ischemic stroke	
12:10-12:30	Bahelková	Cadmium accumulation in organ tissues after inhalation of cadmium-based nanoparticles	
12:30-13:30	Lunch		
<hr/>			
14:00-18:30	Trips and excursions		
19:00-21:00	Dinner		
21:00-21:15	Ceremony awards		

Lecture hall – Kaskáda

Thursday

30
May

		Chair: Greneche	
11:00-11:30	Schünemann	A little journey from single domain particles to single molecule magnets	
11:30-11:50	Jakubowska	Mössbauer studies of three Antarctic meteorites	
11:50-12:10	Mašláň	Air scintillation detector for conversion electron Mössbauer spectroscopy	
12:30-13:30	Lunch		

Conference programme

Lecture hall – Adina

Thursday

Chair: Němec + Vlčková

30

May

11:00-11:30	Profant	From Light to Insight: Exploring Biomolecular Structures via Raman Optical Activity
11:30-12:00	Kapitán	Raman optical activity as an important spectroscopic tool in the study of the structure and interactions of chiral molecules - celebrating 50 years of discovery
12:00-12:20	Jílek	Exploring Mononucleotide G-quadruplexes through Vibrational and Chiroptical Spectroscopy
12:20-12:30	Closing	
12:30-13:30	Lunch	
<hr/>		
14:00-18:30	Trips and excursions	
19:00-21:00	Dinner	
21:00-21:15	Ceremony awards	



Conference programme

Friday

31
May

8:30-9:15	Hof ● Chair: Vičková
9:15-9:45	Mariychuk
9:45-10:05	Lubal
10:05-10:25	Táborský
10:25-11:00	Coffee break

Lecture hall - Vinař

Chair: Kanický

11:00-11:30	Čáslavský
11:30-11:50	Šebesta
11:50-12:10	Vaculovič
12:10-12:45	The End

Lecture hall - Adina

Chair: Miglierini

11:00-11:30	Krehula
11:30-11:50	Kubuki
11:50-12:10	Miglierini

Hotel restaurant

12:30-13:30 Lunch

14:00 Departure



Conference programme

Lecture hall – Vinař

Friday

31
May

Chair: Vlčková

8:30-9:15	● Hof	Are hydration and dynamics factors influencing the activity of enzymes? Insights by combining two fluorescence techniques with MD simulations
9:15-9:45	Mariychuk	Plasmonic metal nanoparticles with a response in the near-infrared region
9:45-10:05	Lubal	Application of sensor arrays for determination of equilibrium constants
10:05-10:25	Táborský	Enhancement of Luminescence Signal by Deuterated Water – Analytical applications
10:25-11:00	Coffee break	

Chair: Kanický

11:00-11:30	Čáslavský	Evaluation of charring influence on the carbon, nitrogen and oxygen stable isotope ratios in archaeobotanical remains
11:30-11:50	Šebesta	Interaction of zinc oxide nanoparticles with Slovak soils and their soil colloids
11:50-12:10	Vaculovič	LA-ICP-MS: an interesting tool for the determination of specific proteins
12:10-12:45	The End	
12:45-14:00	Lunch	

14:00 Departure

Lecture hall – Kaskáda

Friday

31
May

Chair: Miglierini

11:00-11:30	Krehula	Investigations of doped iron oxide nanoparticles by Mössbauer spectroscopy and other techniques
11:30-11:50	Kubuki	The relationship between structure and photocatalytic effect of lanthanide-substituted goethite nanoparticles
11:50-12:10	Miglierini	History of MSMS
12:45-14:00	Lunch	

14:00 Departure

Conference programme

Poster session

P1	P. Matúš	EVALUATION OF KINETIC AND THERMODYNAMIC MODELS FOR METHYLENE BLUE ADSORPTION ONTO SAWDUST OF SPRUCE
P2	N. Vlčková	APPLICATION OF AN ATMOSPHERIC PRESSURE GLOW DISCHARGE-LIKE (APGD) BASED HYDRIDE ATOMIZER TO DETERMINATION OF As AND Se BY AAS
P3	S. Kakalejčíková	A NOVEL VORTEX-ASSISTED LIQUID-LIQUID MICROEXTRACTION BASED ON DEEP EUTECTIC SOLVENT FOR THE SEPARATION, PRECONCENTRATION AND DETERMINATION OF RHODAMINE B IN WATER SAMPLES
P4	Y. Bazel	A GREEN ULTRASENSITIVE FLUORESCENCE DETERMINATION OF ANIONIC SURFACTANTS WITH THE USE OF VORTEX-ASSISTED LIQUID-LIQUID MICROEXTRACTION
P5	A. Hadbavníková	UV-PHOTOCHEMICAL VAPOUR GENERATION OF SILVER: STUDY OF CONDITIONS
P6	M. Svoboda	ATOMIZATION OF HYDRIDE-FORMING ELEMENTS IN ATMOSPHERIC PRESSURE DISCHARGES
P7	V. Vilím	COUPLING OF MINIATURIZED UV-PHOTOCHEMICAL VAPOR GENERATION REACTOR WITH SEQUENTIAL INJECTION ANALYSIS
P8	K. Novotný	PLASMA SPECTROSCOPY IN LASER ABLATION SYNTHESIS OF NANOPARTICLES
P9	S. Zaruba	ASSESSMENT OF MEPS FOR INORGANIC ANIONS DETERMINATION
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ORAL
ABSTRACTS

TRACE ANALYSIS OF METALS AND NONMETALS BY LINE AND CONTINUUM SOURCE AAS COUPLED ONLINE WITH ELECTROCHEMICAL PRECONCENTRATION TECHNIQUES

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The paper presents the most important results of the author's group in the field of atomic spectroscopy.

Trace concentrations of nonmetals such as nitrogen, sulphur, fluorine, chlorine, bromine and a metal (aluminium) in aquatic samples were determined by graphite furnace continuum source high resolution atomic absorption spectrometry (GF-CS-HR-AAS) by making use of formation of diatomic species. The influence of molecule forming elements concentration, chemical modifiers, ashing and atomisation temperatures was investigated. The elaborated procedures were applied for analyses of real water samples.

Electrochemical sample pretreatment has become an excellent tool for improving the sensitivity of atomic spectroscopy in the field of trace and ultratrace metal analysis. Examples of determination of Hg, As, Se, Sb using electrochemical deposition/stripping procedures are discussed. An electrochemical hydride generation approach using a high efficiency flow cell is demonstrated for the determination of antimony in aquatic samples.

Acknowledgements

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IN-VESSEL HEADSPACE LIQUID-PHASE MICROEXTRACTION

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The most common approach in the headspace mode of liquid-phase microextraction (HS-LPME) is to use a microsyringe as a holder of microdrop. This approach combines several steps in sample handling, including separation, preconcentration, and transfer of the concentrate to the instrument. However, it suffers from several factors. The microdrop can grow or shrink in volume, the solvent can separate from the tip of the needle, so the experiment requires careful and complex manual operation. Various approaches were proposed to increase the stability and volume of the acceptor phase. The combination of HS-LPME and UV-Visible spectrophotometry remains difficult primarily because the commonly used acceptor phase volumes are very small (typically 1-3 μL). Recently, a new headspace ME technique termed in-vessel headspace liquid phase microextraction (IV-HS-LPME) was proposed by us [1]. The proposed approach is fully compatible with conventional microcuvettes and instruments used in spectrophotometry. Holding the acceptor phase in a specially designed vessel inside a hermetically sealed vial completely eliminates previously encountered problems with microdrop stability, restrictions on the stirring speed or extraction time, and, above all, volume of the acceptor phase. Since almost any volume of the extraction phase can be placed in the vessel, the proposed approach can in principle be combined with many other analytical methods, such as luminescence, flame AAS, or liquid chromatography. It is important that the proposed approach in terms of the extraction efficiency is not inferior to the methods using a microsyringe to hold the extracting solvent. At the same time, the advantages of HS mode are preserved, such as free choice of solvent, including aqueous solutions, complete separation from matrix components, and absence of memory effects. A new combination of the headspace mode of LPME with an optical probe has been evaluated for the UV-Vis spectrophotometric determination of sulfite [2]. In the HS mode of LPME, only aqueous solutions remain stable in the hole of an optical probe. Holding the acceptor phase inside a vial completely solves the problems of retaining the extracting solvent in the hole of the optical probe.

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COMPLEXATION BETWEEN ACONITINE AND VARIOUS FLAVONOIDES AS POSSIBLE CONCEPT FOR DETOXIFICATION: A SPECTROSCOPIC VIEW ON THE COMPLEX FORMATION

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Monkshood (*Aconitum napellus* L.) is considered the most poisonous plant in Europe. Just two gram of the root can be fatal to humans. Hence, extracts of this plant were used as popular arrow poison and applied for homicides. The toxicity is based on the alkaloid aconitine and some structurally very similar derivatives (hypoaconitine, mesaconitine). Despite the high toxicity of these compounds, extracts of monkshood and related aconitum species have been widely used in traditional healing. They are still used today in Traditional Chinese Medicine in the herbal formula ‘Sini Tang’ (四逆汤). Here, the toxicity of aconitine is reduced by pre-treating the plant parts, which leads to partial hydrolysis of the acetyl and benzyl esters in aconitine. The concomitant administration of liquorice (*Glycyrrhiza uralensis* Fisch.) was identified as a further important contribution to reduce toxicity of aconitine. It is based on the formation of a molecular complex between aconitine and the flavonoid liquiritin from liquorice.[1]

In the present investigation, formation of molecular complexes between aconitine and its corresponding derivatives as well as various flavonoids is examined in further detail. This study is primarily performed using several spectroscopic (NMR, IR, UV), spectrometric (ESI MS) and chromatographic (HPLC) methods for analysis. Combination of the results obtained allows some conclusions about the type of bond formation and the structure of the molecular complex. It becomes clear which functional groups in both molecules cause the complex formation and lead to an unusually high binding constant.

This provides a basis for a future *in silico* calculation of the exact molecular structure and for investigating the toxicity of the complex. A development of possible applications as well as an investigation of the biological significance are also the focus of further studies.

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NMR SPECTROSCOPY OF NUCLEIC ACIDS IN LIVING MAMMALIAN CELLS

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Under in vitro conditions, the structure, dynamics, and interactions of nucleic acids (NA) are sensitive to environmental factors. In-cell NMR spectroscopy provides unique information about the structure and interactions of biomolecules in their native environment inside living cells.

To deliver NA fragments into the cells, three approaches are used: 1. microinjection of NA solutions into *X. laevis* oocytes, 2. reversible permeabilization of the cell membrane using a pore forming toxin, and 3. the electroporation-based approach. Bioreactors are commonly used to avoid problems caused by compromised metabolic activity and cell mortality during prolonged in-cell NMR measurements. A bioreactor is a specialized flow-through NMR cuvette that allows a continuous supply of fresh medium to the cells within in-cell NMR samples.

The in-cell NMR measurements are conducted in a complex heterogeneous environment. The detection of low concentrated nucleic acids inside the cells requires efficient suppression of water signal. To distinguish the signals of the studied NA from those of the cellular background, the investigated NA fragments are often isotopically (¹³C/¹⁵N) and/or covalently (e.g., ¹⁹F) labeled.

In-cell NMR spectroscopy has been employed to assess the effect of nonspecific intracellular factors on the structure of DNA G-quadruplexes, to characterize interactions between a DNA G-quadruplex and a low molecular weight ligand [1], to evaluate the propensity of RNA G-quadruplexes to form high-order structures under in vivo conditions, and to characterize the stability of DNA i-motifs in vivo [2, 3].

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PREPARATION AND CHARACTERIZATION OF POROUS SILVER FILMS BY ION SPUTTERING FOLLOWED BY ION IRRADIATION

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The contribution is devoted to the possibility of the formation of black metals by sputtering of highly pure metals with an intense ion beam of the appropriate energy under a special experimental setup. For the test, a pure silver target (99.99 %) was chosen, which was irradiated with Ar⁺ ions of energy 20 keV at a specific angle of 30°. Sputtering was carried out in the LEIF (Low Energy ion Facility) system, which was assembled in the Laboratory nanomaterials at NPI Rež. The sputtered species (atoms, silver clusters) were directed to the substrate (Si, etc.) at a high angle of about 87° (in the so-called Glancing Angle Deposition setup - GLAD), while the substrate was rotated during deposition (in a way where the Ag deposition was always at an angle of about 87°) with a speed of 3 rpm.

The result of the deposition was a porous Ag layer, the porosity of which was further multiplied by 20 keV Ar⁺ irradiation with high fluences at the levels of 10e16 and 10e17 cm⁻². The prepared nanostructures were subsequently analyzed by several methods (microbeam, RBS, PIXE, SEM, AFM), which showed that it is possible to prepare highly porous Ag nanostructures by ion sputtering of pure target with heavy keV ions and using the specific GLAD arrangement. However, it occurs that the density of the Ag nanoparticles must be increased to match the morphology of typical black metals. This could be realized, for example, by heavy ion bombardment. The first test more or less confirmed this assumption, when the porosity of the Ag film increased significantly after 20 keV Ar⁺ irradiation, but only at high fluences.

Thus, further experimental efforts will be needed to find the optimal way to prepare the highly porous black metals that would be required for their possible applications, e.g., as an essential component of noxious gas sensors [1].

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FINDING CONDITIONS FOR MONOMETALLIC AND BIMETALLIC PLATINUM-CONTAINING NANOCCLUSERS' FORMATION

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Nanosized materials with small diameters are known to be excellent for various applications such as catalysis, sensing of biologically active species, imaging, or for their anti-oxidant and anti-bacterial activity [1]. Noble metal nanoclusters (NCs) consisting of several atoms have been gaining much attention as novel fluorescent markers owing to their optical properties, which include size-dependent emission wavelength. In the present study, we use the green synthesis of monometallic and bimetallic nanostructures where bovine serum albumin is serving as a template, similarly as in one of our previous works [2]. So far, we have investigated the behavior of platinum-containing nanosystems generated by different reducing agents, varying reactant molar ratios and introducing the second metal. Pt NCs show fluorescence emission peak in the range of 450-470nm (370 nm excitation wavelength). Different molar ratios of the reactants have been used to optimize the fluorescent properties of monometallic and bimetallic Pt-containing NCs. The change in the reactants molar ratios affected the fluorescence intensity and position of fluorescence emission maximum. Other factors affecting fluorescent characteristics of these metallic NCs are still under investigation. The as-prepared luminescent NCs can be utilized as contrast agents and/or biomarkers which is going to be tested in the near future. Moreover, they could be implied for catalytic activity and biosensing as known from the literature [3].

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A DECADE OF PORTABLE RAMAN SPECTROMETERS IN MINERALOGICAL STUDIES

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Raman spectroscopy was established as a powerful method for the identification and characterization of minerals in geosciences during the 1990s. Since then, literally thousands of studies have been published, investigating material that has been sampled and carried from the field and analyzed using conventional bench-top Raman instrumentation [1]. The emergence of miniaturized Raman spectrometers in the late 2000s made it possible to conduct investigations outside the laboratory, in indoor and closed environments (such as museums, collections, caves, etc.), as well as fully outdoors (on rocky outcrops, waste heaps, excavations) [2]. However, portable/handheld spectrometers are still not widespread among geologists or mineralogists and their routine use is underrepresented in mineralogical investigations, except for specialized research groups.

Over the course of more than 10 years, we led or collaborated on numerous projects in various fields, including environmental mineralogy and geochemistry, exobiology, gemology, or cultural heritage, where miniaturized Raman spectrometers were used for the primary or supporting method of the non-destructive analysis. Based on this experience, as well as on extensive (and intensive) testing of different miniaturized spectrometers, we would like to present the challenges that can be encountered when working outdoors at real outcrops, in difficult terrain, under daylight conditions, or when measuring non-ideal mineral samples. Various analytical and practical aspects and limitations will be demonstrated on the selected examples of fieldworks involving mineral identification. Furthermore, we will discuss how advancements in miniaturization and the introduction of technically advanced spectrometers in recent years have improved the acquisition of relevant spectroscopic data, solved negative phenomena such as fluorescence, and simplified the use of portable instrumentation for tasks in geology and mineralogy.

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NEW TECHNOLOGY IN RAMAN SPECTROSCOPY: LINE LASER IMAGING AND HIGH THROUGHPUT VIRTUAL SLIT

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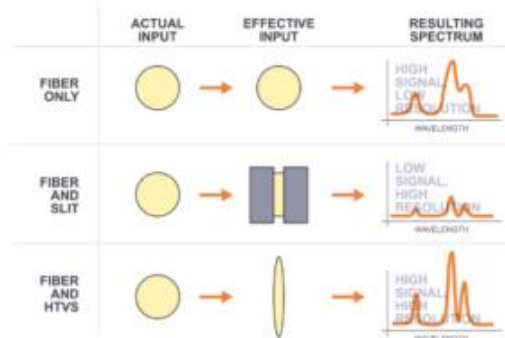
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Although Raman spectroscopy has been a well-established analytical technique for several decades, there are still new and innovative technologies that open up new possibilities and applications in different fields of research.

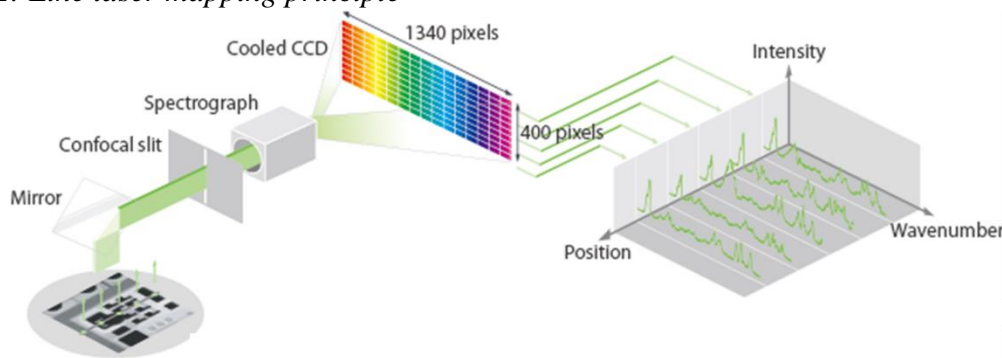
Two of the latest technologies will be presented - the first part of the talk will focus on HTVS (High Throughput Virtual Slit) technology, which allows the use of optical fibers with unmatched sensitivity and spectral resolution. This technology is highly suitable for reaction monitoring and process applications.

Image 1: HTVS technology principle



The second part focuses on a breakthrough in chemical Raman imaging - line laser imaging technology. This technology combines a line laser with a large CCD detector and allows to collect 400 spectra simultaneously. This results in extremely fast data acquisition with significantly higher sensitivity compared to other existing Raman imaging instruments. This technology allows also highly effective and fast deep profiling.

Image 2: Line laser mapping principle



LA-ICP-MS: A KEY TO DETAILED IMAGING OF TRACE ELEMENTS IN GEOLOGICAL SAMPLES

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Inorganic analysis of geological samples is foundational to geochemistry, traditionally involving bulk analysis after sample decomposition or water analysis using diverse techniques. However, in-situ analysis of solid samples, such as Backscattered Electron (BSE) imaging, X-ray microanalysis, and notably Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS), has transformed our approach to these studies. These surface techniques enable detailed imaging of selected sample areas, offering a more granular view of elemental distribution compared to traditional spot analyses. Specifically, LA-ICP-MS has become integral for creating elemental or isotopic maps, crucial for investigating mineral heterogeneity, elemental mobility, and the chronological dating of geological processes [1].

By performing scanning ablation across defined areas, LA-ICP-MS achieves high-resolution images of elemental or isotopic distributions under optimized conditions, with key factors such as ablation spot size, scan speed, dwell time, number of measured isotopes, and data evaluation procedures affecting the method's success. This advanced imaging capability is essential for deciphering the geological and environmental histories represented by the samples [2].

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SPECTROSCOPICAL APPROACH FOR STUDYING BIOLOGICAL SHIELDING CONCRETE

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Biological shielding concrete serves as a crucial protective barrier against ionising radiation but encounters challenges from neutron and gamma radiation, as well as thermal stresses. Despite its critical role, comprehensive studies on the impact of concrete irradiation on its properties are limited, revealing significant gaps in current knowledge from the perspective of local sources. Understanding the degradation mechanisms affecting nuclear power plant structures, particularly within containment units, is essential. This has drawn considerable attention from international organisations, national regulators, and research entities within the nuclear industry because the extension of operational licenses for nuclear power plants is a notable global issue [1].

In the context of biological shielding concrete, spectroscopy is a valuable tool for researchers to comprehensively investigate the concrete component materials' elemental composition, crystalline phases, and bonding properties. Acquired spectroscopic data can guide the refining process of concrete formulas to improve radiation shielding efficacy. Various additives, aggregates or cement pastes could be analysed using many available modern spectroscopic techniques. Nevertheless, challenges arise when handling highly irradiated samples that are inherently radioactive. In the case of both pre- and post-irradiation research, Raman spectroscopy offers a rapid and non-invasive method for conducting structural-chemical analyses, particularly beneficial in evaluating radiation-induced amorphisation [2] or crystal-bound water loss in minerals (aggregates) and materials. When integrated with SEM-EDX and X-ray diffraction techniques, it enables the correlation of data sets like the degree of radiation damage, alterations in structure, cell volume expansion, and shifts in chemical composition.

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LEAD ISOTOPIC ANALYSIS: BACK TO BASICS, POTENTIAL OF CURRENT ANALYTICAL TECHNIQUES & VISIONS FOR FUTURE IMPROVEMENTS

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Isotopic analysis has become a trend in the field of analytical chemistry and has been widely used in many application fields [1]. Few techniques draw the attention of analytical chemists for quite a long time now – Thermal Ionization Mass Spectrometry (TIMS), Secondary Ion Mass Spectrometry (SIMS) [2], Inductively Coupled Plasma Mass Spectrometry (ICP-MS) [3], Electron Microprobe Analysis (EMPA). Each of these techniques provides different approach, advantages, and disadvantages to isotope ratios determination – in the case of EMPA we consider only the dating of geological samples in this context – and will be discussed during the lecture.

In this presentation, we would like to point out the lead isotope ratio analysis using ICP-MS method with quadrupole mass analyzer (ICP-(Q)MS) together with the comparison of single-collector and multi-collector (MC) ICP-MS instrumentation in the context of accuracy and precision within various applications. Although some publications strictly advise the use of (MC) ICP-MS, for some interpretations, single-collector ICP-MS might be sufficient [4]. Our results show that with ICP-(Q)MS a compromise must be made during the isotope ratio analysis while preferring accuracy over precision or vice versa but resulting in lower price and wider availability to users who already own the ICP-(Q)MS instruments. We will also introduce ideas for future method developments.

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LOCAL STRUCTURAL AND MAGNETIC PROPERTIES OF FE CONTAINING NANOARCHITECTURE

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After a brief presentation of the main characteristics of nanoarchitectures, we review the various questions aimed to better understand their structural and physical properties. We illustrate this strategy with some examples based on results obtained by ^{57}Fe Mössbauer spectrometry, a local probe technique well suited to the study of these complex Fe-containing nanomaterials. We show also that this fundamental approach was necessary to better understand the relationship between the morphology of nanostructures and their physical and chemical properties and also to characterize the structural and magnetic properties of highly complex nanoarchitectures including nanoparticles, hollow nanoparticles, nanocomposites and nanoaggregates.

SPATIALLY RESOLVED MATERIAL ANALYSIS USING A COMBINED LA-ICP-MS AND LIBS PROCEDURE

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Laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS) and laser-induced breakdown spectroscopy (LIBS) are powerful techniques for spatially resolved elemental analysis. While LA-ICP-MS offers better sensitivity down to the ng g⁻¹ level, LIBS allows to measure almost every element of the periodic table, including elements such as H, C, N, O, and F, which are not easily accessible by ICP-MS. Attributes that make these two techniques attractive for imaging and depth profiling applications are fast sample throughput, no or minimal sample preparation and applicability to all kinds of solid samples. Since the signal generation of these analytical methods relies on firing a focused laser beam on the sample surface, they can be merged into a combined measurement method, where element specific information from one sample location can be acquired simultaneously by both techniques. Thereby, a more comprehensive sample characterization is enabled. However, to tackle the permanently rising demands in spatially resolved sample characterization, continuous development of this approach is inevitable.

In this contribution we developed a combined LA-ICP-MS & LIBS procedure. Utilizing a 193 nm ns ArF excimer laser for sample ablation enabled fast mapping experiments with enhanced resolution. Measurement of single pulse responses allowed simultaneous detection of metals and non-metals in various sample types. Applicability of developed procedures is demonstrated by the analysis of microplastics and protective coatings as examples for research questions from the fields of environmental and material sciences.

MÖSSBAUER AND XRD OBSERVATION OF THE EFFECT OF SWIFT HEAVY ION IRRADIATION IN NANO-MAGHEMITE

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Our present research is part of a series of investigations, in the frame of an international collaboration, to study radiation induced effects of swift heavy ion irradiation in metals, alloys, nano-materials, like nano-iron-oxides, etc., which resulted publications such as [1,2]. In the present work ⁵⁷Fe transmission Mössbauer spectroscopy and X-ray diffractometry (XRD) were used to study the effect of 160 MeV ¹³²Xe ion irradiation with fluences of 5×10^{13} and 10^{14} ion cm⁻² on sol-gel prepared maghemite nanoparticles. The non-irradiated nano-maghemite showed poorly resolved magnetically split room temperature (RT) Mössbauer spectra, typical relaxation spectra, indicating superparamagnetic state at RT. The swift heavy ion irradiation caused significant fluence dependent changes in the spectral shapes of Mössbauer spectra corresponding to the change in the superparamagnetic state of nano-maghemite. XRD of the irradiated maghemite nanoparticles revealed a significant broadening of the corresponding lines compared to those of non-irradiated ones, indicating a decrease of crystallite size, accordingly to the change in the superparamagnetic state. The results are discussed in terms of the defects induced by the swift heavy ion irradiation and corresponding changes related to the change in particle size and consequently in the superparamagnetic state induced by irradiation.

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MICROSCOPIC PHENOMENA IN Fe-Cr ALLOYS

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Fe-Cr alloys have been both of scientific and industrial interests. The former results from their interesting magnetic properties and the latter from their significance in the steel making industry. Both these aspects can be efficiently investigated by Mössbauer spectroscopy (MS). This contribution will be mainly concerning the latter. The industrial importance of the Fe-Cr alloys originate from the fact that the alloys containing at least ~10.5 at. % Cr is stainless. Consequently, Fe-Cr alloys have been used as the major component of several grades of stainless steels, in particular ferritic and martensitic (F/M) ones. These steels because of their excellent properties like resistance to high temperature corrosion, low swelling and high strength, have been used as structural materials for manufacturing various devices like, for example, heat exchangers, turbines, pipes, can work at service at elevated temperatures and in aggressive atmosphere. Consequently, the devices have been used in such branches of industry like power plants, including nuclear ones, oil refineries to name just few. However, their functional qualities deteriorate with time of usage. Processes and mechanism responsible for such worsening occur at microscale and the major ones are radiation damage and hardening. The latter can have two reasons: (a) phase separation into Fe-rich (α) and Cr-rich (α') phases and it is known as “475°C embrittlement”, and (b) precipitation of σ -phase. Both phenomena can be understood in terms of the crystallographic phase diagram of the Fe-Cr system. They can be successfully and quantitatively studied by means of MS. Examples illustrating the application of MS to the following issues pertinent to the subject will be addressed and discussed:

- Kinetics of the phase separation
- Energy of activation
- Limit of solubility of Cr in iron and Fe in chromium
- Kinetics of σ precipitation
- Short-range ordering (SRO)
- Effect of plastic deformation on SRO
- Effect of irradiation on SRO

The experimentally obtained results will be compared with relevant theoretical predictions. More detailed information can be found elsewhere [1].

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STRUCTURE ANALYSIS OF SURFACE-TREATED CL20ES SAMPLES BEFORE AND AFTER ANNEALING

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Additive manufacturing, a fast-growing area of 3D metal printing, enables low-cost, low-volume production and simplifies the manufacture of complex parts. Unlike conventional techniques, additive methods often involve melting the powder material using a laser (e.g. selective laser melting, SLM). The printing process is usually carried out in an inert atmosphere. In the post-process, the manufactured parts are sandblasted to remove imperfectly sintered surface layers and subsequently annealed to remove significant internal stresses created during printing. This annealing process is conducted under a variety of conditions: temperatures below 1000°C, annealing intervals varying according to component size and desired mechanical properties, and various atmospheres. In the context of diverse treatment processes, additional phenomena can arise that diverge from those observed in conventional techniques.

Our previous studies have mainly focused on the analysis of input powders [1] and the annealing of as-prepared samples [2]. In this contribution, we further explore the topic by examining the mechanically surface-treated components made of CL20ES steel. During the tempering of as-prepared components [3], significant chromium segregation towards the surface was observed. Interestingly, the surface segregation was significantly reduced in ground and polished samples. Under the chosen tempering protocol (550°C for 36 hours in air) almost no surface segregation occurred. High chromium content occurred again at the surface under greater annealing temperature (1000 °C for 36 hours in air). As a result, the surface properties of the treated component may differ slightly from those of the untreated component. While the surface protection against corrosion may be changed due to the new phases on the surface, we expect the mechanical strength to be higher [4]. The SLM-printed and mechanically treated (ground and polished) samples of CL20ES steel were studied using Mössbauer spectroscopy, X-ray diffraction, scanning electron microscopy, and energy dispersive spectroscopy.


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PRECIPITATION OF ODS STEELS AFTER LONG-TERM ANNEALING

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Oxide dispersion strengthened (ODS) steels are key alloys used in nuclear installations. Steels with chromium content of up to 10 wt. % are suitable due to their advantageous properties and these alloys are used for the construction of technological devices in the primary circuit of nuclear power plants. From other studies, it can be concluded that chromium has anti-corrosive properties due to formation of a passivation layer, which results in lower activation of the material by thermal neutrons. Macroscopic properties are determined by their microstructure and therefore the description of the microstructure is important. Transmission ⁵⁷Fe Mössbauer spectroscopy and atom probe tomography were used to describe microstructural features of the investigated materials. In this way, information about the physical and/or chemical environment of the resonant atoms can be achieved. The obtained spectral parameters reach saturation values from which the solubility limit of chromium in iron can be determined. In Cr-rich phase, the solubility limit can be estimated from the value of spectral parameters of the single-line in the spectrum annealed for the longest time. The suggested procedures are subsequently applied to the case studies of stainless steels suitable for the construction of various components of the III+/IVth generation of nuclear reactors (including fast and fusion reactors).

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ADSORPTION OF SOME METAL CONTAMINANTS IN WATER USING AKAGANEITE NANOPARTICLES: SPECTROSCOPIC AND KINETIC STUDIES

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Akaganeite, β -FeOOH, nanoparticles have long been employed as adsorbents for eliminating various contaminants from polluted water. This is due to its availability, extensive specific surface area, the existence of tunnel sites, and the multitude of synthesis options featuring modified surfaces [1-3]. In this work, we compare the absorption performance of both pure and co-precipitated akaganeite nanoparticles to eliminate Pb²⁺, As³⁺, As⁵⁺, Sb³⁺ and Hg²⁺ in aqueous solutions [3]. The absorption kinetics were modeled by using 6 nonlinear equations reported in the literature [4]. It was found that akaganeites co-precipitated in presence of cations [2] had better adsorption capacities than pure akaganeites. The highest adsorption capacity values for a particular pollutant were found to be unaffected by the choice of cation employed for co-precipitating akaganeite. These results suggested that the morphological characteristics of akaganeites play a crucial role in dictating their adsorption capabilities. Sb³⁺ was the fastest adsorbed pollutant, whereas Hg²⁺ was the slowest one. Elovich and simplified Elovich models properly described the experimental kinetic data for Sb³⁺, whereas the Bangham model properly fit the kinetic data for Hg²⁺ [3]. On the other hand, the isomer shifts and quadrupole splittings for the two doublets of the 300 K Mössbauer spectra for all samples, before and after adsorption, were rather similar. In contrast, 77 K Mössbauer spectrometry showed small variations in some of the hyperfine parameters of akaganeite after adsorption of different pollutants in comparison to akaganeite before adsorption [3].

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MÖSSBAUER, XRD AND SEM/EDX SPECTROSCOPIC STUDY OF DC MAGNETRON SPUTTERED AISI 304 STAINLESS STEEL FILMS

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The investigation of 200 nm – 2 μm thick films derived from AISI 304 stainless steel via DC magnetron sputtering presents insight into their magnetic and structural characteristics. This study investigates the transition from the traditionally non-magnetic FCC phase of austenite (γ -Fe) in AISI 304 steel to a primarily BCC single-phase (α -Fe) during the deposition process undergoing the martensitic transformation. The resulting films exhibit ferromagnetism at room temperature. Study emphasizes the importance of detailed preparation process description. Films characterization utilized techniques such as ⁵⁷Fe Mössbauer spectroscopy in transmission, conversion electron and conversion X-ray arrangements, X-ray powder diffraction and scanning electron microscopy. Some results of the induced transformation of these films will be also presented.

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ENHANCING MÖSSBAUER SPECTROSCOPY FOR EFFICIENT QUALITY CONTROL IN METALLURGICAL INDUSTRIES

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Mössbauer spectroscopy, despite its potential for providing valuable insights into iron-containing sample composition, remains underutilized in the metallurgical and steel industry. This reluctance stems from various challenges, including legislative hurdles related to ionizing radiation sources, the absence of internationally recognized norms, and the time-consuming nature of measurements, particularly concerning low iron content samples. Our efforts focus on the third problem, the measurement time optimization through Bayesian statistical methods.

The primary industrial application of Mössbauer spectroscopy lies in the quality control of incoming raw materials and manufactured products, where familiarity with the material is established. Therefore, the following workflow can be implemented. Initially, a high-quality spectrum of material or product is obtained. This defines the model to be used. Quality control for subsequent batches involves capturing periodical spectra (e.g. every minute) and fitting them to the established model using Markov Chain Monte Carlo (MCMC) methods. Every minute, the composition of the sample is estimated together with the uncertainty of the estimate (e.g. the probability that the sample contains less than 5 % of austenite). This allows us to stop the measurement process as soon as the desired accuracy is achieved, thus optimizing the quality control process.

Our work aims towards the successful deployment of this approach in the laboratory of a partner company. The dedicated user interface, methods, and results showcasing the effectiveness of the proposed method in streamlining quality control processes within metallurgical industries will be presented.

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FAST ⁵⁷FE MÖSSBAUER AUSTENITEMETER

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⁵⁷Fe Mössbauer spectroscopy has a unique ability to non-destructively analyse different iron-containing materials – distinguishing various iron-bearing compounds and the possibility to study phase composition in steels. This feature would be attractive for a metallurgical industry, where steel phase composition control is a crucial task. Unfortunately, Mössbauer spectra accumulation is a highly time-consuming process. Even with a strong radiation source (with activity in GBq), it is a matter of units or tens of hours. This obstacle can be remedied. Long measurement time is needed to ensure a good statistical quality of a spectrum. However, if we only need to know the percentage of different phases (in our case ferrite vs. austenite; i.e. residual austenite), we can reduce the measurement time by recording a few specific points in the spectrum. In the upcoming study, we will introduce the solution for optimized fast analysis of austenite occurrence in steels, some predicted in [1], and based on the specific approach of radiation source synthesis [2,3]. The obtained results indicate the possibility of constructing a specialized Mössbauer spectrometer.

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FROM ISOTOPE FRACTIONATION TO CHEMICAL SPECIATION OF BIOLOGICALLY RELEVANT SUBSTANCES

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Modern measurement systems using plasma based techniques, complement by elemental and molecular mass spectrometry could be considered as a powerful tool that provides unique information about the chemical composition of the tested systems. Several examples of projects carried out with medical doctors, in which the results of speciation studies support the determination of metabolic processes, as well as the transport routes of substances of biological importance will be discussed.

The study of the fractionation of elements with more than one stable isotope indicates the isotope fractionation during transport through cell membranes. Another project is focused on the study of the biotransformation of various elements of biological significance, including magnesium, chromium, strontium, iron, copper, and selenium. The example of biotransportation of those elements in the brain, ovaries, and kidneys will be given. Another example of the studying of the metabolism of fluorinated drugs and the phenomenon of jumping fluoride from small drug molecules to proteins will be also presented.

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SURFACE ENHANCED RAMAN SPECTROSCOPY IN BIOANALYTICS

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Raman spectroscopy is a powerful analytical tool in biomedical application schemes; however, its limitation is associated with the intrinsic weak Raman effect. This is overcome by applying powerful plasmonic nanostructures creating the surface enhanced Raman spectroscopy (SERS) technique. SERS is applied to identify and estimate trace concentration of biomolecules such as drugs and its metabolites or biomarker even in complex matrices. [1, 2] As an example, the SERS technique was applied to estimate the antibiotic ciprofloxacin in pharmaceutical formulations. In the case of simple matrix compositions, e.g. sodium chloride infusion solutions, Raman spectroscopy can be applied in the required concentration range. For formulations with high Raman background signal, a dilution by 1:5000 was applied and the recorded SERS spectra were only dominated by the contribution of the target ciprofloxacin, which is associated with the strong affinity of this drug towards the metal sensing surface. [3] Furthermore, we illustrated the SERS-based detection of pyrazinoic acid (POA), a metabolite of the tuberculosis-relevant prodrug pyrazinamide (PZA). To be specific for POA, gold nanoparticles equipped with a Prussian blue modification were applied, complexing the POA molecules via Fe (II). This scheme has a high potential in assessment of PZA resistance in *M. tuberculosis* bacteria, as only sensitive bacteria convert PZA into POA. [4] To illustrate the potential of SERS in therapeutic drug monitoring, the antibiotic ceftriaxone was spiked in fresh blood plasma samples as well as microdialysates and the role of proteins within this detection scheme is discussed. In microdialysate samples, detection down to 1.4 μM is achieved. [5] Finally, we studied the SERS signature of saliva to verify the detection of salivary biomarkers, i.e. interleukin-8 and lysozyme by combining SERS with molecular dynamics simulations. [6]

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TIP-ENHANCED RAMANA SCATTERING – OLD STORIES AND NEW DEVELOPMENTS

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For 25 years tip-enhanced Raman scattering (TERS) allows structurally sensitive analysis of surfaces with nanometer and sub nanometer lateral resolution. In this presentation, after a short introduction to the methodology, an overview of different applications in our research group will be provided. Namely, results on problems in bio-materials [1], polymer nano particles [2], and surface catalysis [3] will be shown with an emphasis to the high spatial resolution and the particular challenges related to the extreme resolution.

While molecularly sensitive surface analysis with high resolution is one of the main strengths of the technique, specifics of the technique also allow to gain information to other parameters of the specimen with similar or equal resolution. One example will be related to the localized temperature detection via Stokes-Anti-Stokes ratios under plasmon enhanced conditions [4]. If time permits recent progress on signal/focus optimization of laser beams using near-field optics and TERS information will be shown.

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RECENT ADVANCES IN PHOTOCHEMICAL VAPOR GENERATION OF SEVERAL TECHNOLOGY-CRITICAL ELEMENTS

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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 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, mainly formic or acetic acid.

This presentation will be devoted to our most recent achievements in the PVG of several new analytes [1,2] belonging to the so-called group of technology-critical elements (TCEs). Despite increasing use in modern technologies, these elements are extremely rare in nature and require ultrasensitive detection methodologies. Evidence will be presented of efficient coupling of PVG to an inductively coupled plasma mass spectrometer to provide excellent detection power for determination of several TCEs (e.g., Ru and Ir), even in complex matrices such as seawater (limits of detection in single units to tens of ppq). Details relevant to optimization of PVG conditions will be highlighted. Attention will also be paid to efficient PVG of Ru, Re, and especially Ir from dilute formic acid media (≈ 0.01 M) and its related mechanistic aspects [3]. Finally, recent attempts to identify the form of generated volatile species (metal carbonyls) using alternative ionization techniques combined with mass spectrometry will be discussed.

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APPLICATION OF SIX-STEP SEQUENTIAL EXTRACTION FOR DETERMINATION OF ZINC FRACTIONS IN PADDY SOILS

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The extractability and quantitative knowledge of how zinc (Zn) is bound in the soil supply essential information on the mobility, bioavailability or deficiency of Zn regarding to the different soil characteristics. As Zn is present in the soil in several chemical forms or bound to various fractions (e.g., organic matter, carbonates), its total content does not give enough information about its mobility and bioavailability for plants. Therefore, in our study, the mobility and availability of Zn in the alkaline paddy soils collected from the Terzeria farm, Calabria (Italy) were investigated using six-step sequential extraction, a modified BCR method. This method allowed us to fractionate zinc into (1) water soluble and exchangeable fraction, (2) fraction bound to carbonates, (3) fraction bound to Mn oxides, and (4) amorphous or (5) crystalline Fe minerals, and (6) oxidizable fraction (bound to organic matter and sulfides). The total concentrations of Zn and the concentration in different fractions after extraction were determined by flame atomic absorption spectrometry (FAAS). Soil samples were collected from different fields in one area, which are cultivated using crop rotation system (rice, forage and pomegranate). Even though the analyzed soil samples have similar chemical characteristic (slightly alkaline pH value), the different cultivation method resulted in alteration of the Zn pools.

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LASER INDUCED FLUORESCENCE: A RELIABLE TOOL FOR DIAGNOSTICS AND DEVELOPMENT OF HYDRIDE ATOMIZERS

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Hydride generation (HG) is a useful sample derivatization step in trace element analysis. It reaches almost quantitative and matrix-free analyte introduction into the atomic spectrometric detector. Various hydride atomizers based on flame, heated quartz tube (QTA) or plasmas are employed in atomic absorption spectrometry (AAS). QTAs are the most common hydride atomizers in AAS offering high sensitivity universally for all hydride forming elements including As, Se, Te, Sb, Bi, Sn and Pb. The only exception is Ge, with sensitivity lower by two orders of magnitude. Recently, ambient plasmas such as volume dielectric barrier discharges (DBDs) have been reported to be an alternative to QTAs. However, significant differences in sensitivity were found among individual hydride forming elements. The signals of Se, Te and Sb are comparable in DBD and QTA while those of Pb and Sn are significantly lower in DBDs. Analogously to QTA the sensitivity of Ge determination is low in DBD as well.

Laser induced fluorescence (LIF) was employed as a useful diagnostic tool capable of determination of spatial distribution of free analyte atoms in the DBD atomizers as well as quantification of their absolute concentration leading to assessment of atomization efficiency. The results found by LIF are in perfect agreement with the observations made by AAS. Homogeneous distribution of free analyte atoms in the whole discharge area and atomization efficiency in high tens of percent was observed for Se, Sb and Te. On the contrary, the occurrence of free atoms was restricted only to the central part of the DBD discharge in case of Pb, Sn and Ge with atomization efficiency being quantified to ca 20% (Pb, Sn) and even only 5% for Ge, respectively. Hydrogen radicals were, as important species responsible for hydride atomization in QTA and DBD, detected by two photon absorption LIF (TALIF). Their distribution in the discharge area is homogeneous with concentration reaching 10^{21} m^{-3} H, i.e. several orders of magnitude higher than requested at typical analyte concentration levels. The variability in sensitivity for hydride forming elements in the DBD atomizer can be explained by element dependent decay kinetics of free atoms by deposition. Also other plasma atomizer designs, namely RF plasma jet or the atmospheric pressure glow discharge-like (APGD) plasma were investigated by LIF regarding their capability to dissociate Se and Ge hydrides while TALIF was employed for determination of H radicals.

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PLASMA ASSISTED VAPOR GENERATION OF PLATINUM GROUP ELEMENTS

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In this work, preliminary results achieved with a new plasma assisted vapor generation (PAVG) as an alternative sample introduction technique for ICP-MS will be presented [1]. The PAVG was constructed using a tubular dielectric-barrier discharge (DBD) and a Meinhard type nebulizer (MicroMist) as liquid sample introduction into the DBD. An in-lab built power source was used for plasma generation. The platinum group elements (PGEs) were chosen for the preliminary studies, including Ir, Pd, Pt, Rh [2], Os and Ru. The early development of this new PAVG was focused mainly on the proper and robust construction of the PAVG generator, the size of the external copper electrode and its position relative to the nebulizer tip and the power source modulation/input voltage for a stable plasma generation. ICP-MS/MS was utilized as a detection technique using He as a collision gas.

Once the device exhibited a robust performance, the research was subsequently focused on the examination of various conditions affecting the efficiency of vapor generation. Mineral acids (HNO₃ and HCl) and organic acids (acetic acid and formic acid) in different concentrations were tested as the carrier medium. The observed effects for individual PGEs differed significantly, suggesting the optimal conditions for vapor generation is different depending on the element. Using Cs as the element, which is assumed not to produce any volatile species by the PAVG, it appears that an important part of the measured analytical signal is obtained due to an increment in the sample aerosol transfer efficiency by the PAVG rather than in a generation of volatile species. Regarding generation of truly volatile species by the PAVG, the results are especially promising for Ir and Rh. The constructed prototype of the DBD device will be the base for future research on this topic.

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SPATIALLY RESOLVED MATERIAL ANALYSIS USING A COMBINED LA-ICP-MS AND LIBS PROCEDURE

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Laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS) and laser-induced breakdown spectroscopy (LIBS) are powerful techniques for spatially resolved elemental analysis. While LA-ICP-MS offers better sensitivity down to the ng g⁻¹ level, LIBS allows to measure almost every element of the periodic table, including elements such as H, C, N, O, and F, which are not easily accessible by ICP-MS. Attributes that make these two techniques attractive for imaging and depth profiling applications are fast sample throughput, no or minimal sample preparation and applicability to all kinds of solid samples. Since the signal generation of these analytical methods relies on firing a focused laser beam on the sample surface, they can be merged into a combined measurement method, where element specific information from one sample location can be acquired simultaneously by both techniques. Thereby, a more comprehensive sample characterization is enabled. However, to tackle the permanently rising demands in spatially resolved sample characterization, continuous development of this approach is inevitable.

In this contribution we developed a combined LA-ICP-MS & LIBS procedure. Utilizing a 193 nm ns ArF excimer laser for sample ablation enabled fast mapping experiments with enhanced resolution. Measurement of single pulse responses allowed simultaneous detection of metals and non-metals in various sample types. Applicability of developed procedures is demonstrated by the analysis of microplastics and protective coatings as examples for research questions from the fields of environmental and material sciences.

ANALYSIS OF METALS BY ATOMIC SPECTROMETRY

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Agilent atomic spectrometers (AAS, ICP-OES, ICP-MS) have been the best-selling spectrometers on the market in the Czech Republic and worldwide for many years. They form a solid foundation of instrumentation for metal analysis in a wide range of thriving commercial, research and surveillance laboratories. They have unrivalled technologies whose functionality is tested in detail every day, even on the most complex matrices. Yet they excel in ease of use and can provide users with much more information about the samples being measured. Easy, fast, cheap. They represent very good value for money. The details that make Agilent spectrometers unique are countless. Now also with a high degree of automation thanks to the brand new Agilent ADS dilution unit. But in this talk, you will briefly learn about the most important ones and get an idea of why Agilent atomic spectrometers are so popular.

Atomové spektrometry Agilent (AAS, ICP-OES, ICP-MS) jsou již řadu let nejprodávanějšími spektrometry na trhu v České republice i ve světě. Tvoří pevný základ přístrojového vybavení pro analýzu kovů v celé řadě prosperujících komerčních, výzkumných a dozorových laboratoří. Disponují bezkonkurenčními technologiemi, jejichž funkčnost je každodenně detailně testována i u těch nejsložitějších matic. Přesto vynikají snadným používáním a mohou uživatelům poskytnout mnohem více informací o měřených vzorcích. Snadné, rychlé, levné. Představují velmi dobrý poměr ceny a výkonu. Detailů, které činí spektrometry Agilent jedinečnými, je nespočet. Nyní také s vysokým stupněm automatizace díky zbrusu nové řídící jednotce Agilent ADS. V této přednášce se však stručně seznámíte s těmi nejdůležitějšími a získáte představu o tom, proč jsou atomové spektrometry Agilent tak oblíbené.

LASER-INDUCED BREAKDOWN SPECTROSCOPY IN ANALYSIS OF ALGAE

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Green algae *Desmodesmus subspicatus* are single cell freshwater organisms capable of heavy metals accumulation from water. They are analyzed with Inductively Coupled Plasma Mass Spectrometry (ICP-MS) but the parent solution with algae is filtered, the filter with an algae sediment is decomposed and the resulting solution is analyzed with ICP-MS. However, such procedure is laborious and time-consuming. An alternative technique is Laser-Induced Breakdown Spectroscopy (LIBS) with a Czerny-Turner spectrometer in a double pulse (DP) 1064-1064nm configuration [1]. It is sufficiently sensitive to the heavy metals concentrations of about tens of ng cm⁻² on the filter surface. A semiquantitative analysis is then possible. Besides, some interesting facts about LIBS of the cellulose filter were revealed. Contaminated algae show monotonous decrease of lines intensities with number of used layers of adhesive tapes for fixing the filter to a microscope glass while blank and non-contaminated samples do not. Also the total emissivity, electron number density and the matrix elements lines are less intensive on the blank than on the contaminated sample. Analogical behaviour shows also plasma shockwave from shadowgraphy experiments. Behaviour of the analyte and the matrix lines is more similar if their signal-to-noise ratio is high or they have similar excitation energies which can be important for possible internal standardization.

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ACOUSTIC/OPTICAL EMISSION SPECTROSCOPIC HYPHENATED DATA FROM LASER-INDUCED PLASMAS. FROM THE CONCEPT TO THE SCENE

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The relevance of laser-induced plasmas acoustics (LIPAc) investigations has skyrocketed in recent times, raised by NASA's mission Mars 2020 research with the Mars Microphone, one of the five measurement techniques of SuperCam to record the first sounds on the planet, consisting of wind, dust devils, rover noises, and the laser zaps over geological matter to support the LIBS investigation to obtain unique properties [1]. While LIPAc signal has been succinctly studied and applied to LIBS signal, preferably as a normalization asset to alleviate the shot-to-shot optical signal instability inherent to generated plasmas, only some minor systematic studies on the background of the phenomenon have been conducted [2].

Research herein focused on the evaluation of factors that may condition LIPAc signal, from geometrical (diameter, thickness) and physical (light absorption, porosity) sample-related traits, as well as surrounding-related (type of terrain) and operational conditions (microphone coordinates to the target and to the floor). In addition, effects on LIPAc signal were evaluated when different wavelengths and focal conditions were used to generate plasmas and when recorded with miscellaneous types of microphones. From all this, LIPACs-based mappings were demonstrated to be useful in reflecting the surface morphology of solid targets.

Using all this knowledge on LIPAc, recently, the experiments were moved inside a thermal-vacuum chamber (TVC), a facility that allows mimicking planetary environments to evaluate LIPAc signal performance under different pressure and temperature levels, as well as under distinct atmosphere compositions. In short, complete research aimed at contributing to potential uses of the LIBS-LIPAc combination in future space missions.

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IMAGING OF URANIUM ORES BY LASER INDUCED BREAKDOWN SPECTROSCOPY (LIBS)

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One of the fundamental issues in the Czech Republic is finding a suitable and safe place to store radioactive waste from a nuclear power plants. This issue was the topic of the GeoBarr project, where one of its parts was research on the mobilization of uranium in the environment. For this purpose, rich natural deposits are offered as an analogy for the behavior of uranium in the environment. Within this project, chemical imaging of natural uranium ore samples was investigated [1,2].

The first part of this work combines two chemical imaging methods, LIBS and LA-ICP-MS (Laser-Induced Breakdown Spectroscopy and Laser Ablation with Inductively Coupled Plasma Mass Spectrometry). Fast LIBS scanning made it possible to perform analysis across the whole sample, containing three different parts (metasomatite; carbonate and massive uraninite vein). The LA-ICP-MS method focused in detail on interesting areas in individual parts with a high resolution. A two different uranium mineralization types and their genetic relationship were revealed by this combination of large maps obtained by LIBS accompanied by highly detailed LA-ICP-MS imaging demonstrated on the analyzed sample [1].

The second part of the work uses the capabilities of the LIBS method to detect oxygen and hydrogen. This is a significant advantage of LIBS compared to many other methods including microprobe analysis. Based on this fact LIBS can help distinguish the oxidation state of uranium or content of crystal water. That was demonstrated on the uranium ore sample which contained phases with different uranium forms – uraninite (UO₂) and uranophane (Ca(UO₂)₂(SiO₃OH)₂·5H₂O) [2].

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EXPOLORING THE ENVIRONMETNAL ROLE OF ARSENIC SPECIATION IN MACROFUNGI

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Terrestrial fungi are significant organisms in the forest environment, playing an important role in biogeochemical cycles of trace elements. Fungi are capable of mobilizing various elements from soil and bedrock, making them accessible to other organisms [1]. One such element is arsenic. It is known that macrofungi usually contain various arsenic compounds, and speciation is variable between different mushroom species [2]. However, it is not clear if the macrofungi are metabolizing arsenic to different compounds themselves, if it is induced by microorganisms or if they just accumulate them from the surrounding environment.

These questions will be discussed in the lecture based on results obtained through the combination of analytical and microbiological methods. From the perspective of analytical chemistry, the high-throughput method for determination of arsenic species using ion-pair reversed phase liquid chromatography and inductively coupled plasma mass spectrometry will be presented. This method was used to study the arsenic metabolism in mycelia of *Hebeloma* mushrooms cultivated in arsenic-enriched medium. It was found that mycelia are capable of transforming arsenate from growth medium into a variety of compounds (e.g., dimethylarsinic acid, arsenobetaine, and trimethylarsine oxide), as well as releasing some of these compounds back into the growth medium. This was supported by subsequent experiments in which genomic sequences of specific arsenic efflux transporter ACR3 from tested *Hebeloma* mushrooms were inserted into arsenic-sensitive *Saccharomyces cerevisiae* mutants. These yeasts cultivated in dimethylarsinic acid or trimethylarsine oxide containing medium accumulated and metabolized a portion of these compounds into other organic species of arsenic. Moreover, their total contents in cells were lower compared to control yeasts without inserted transporter genes. This suggests that ACR3 transporters are probably able to transport organic arsenic species out of the cells. Thus, it seems that macrofungi may play a more significant role in biogeochemical cycle than previously assumed. However, a detailed explanation of all mechanisms requires further research.

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SIMULTANEOUS DETERMINATION OF PB, AL, AND FE IN THE ANALYSIS OF ANTARCTIC TERRESTRIAL FLORA USING HR-CS GF-AAS

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Current instrumentation for high-resolution continuum source atomic absorption spectrometry (HR-CS AAS) allows for observation of the spectral line and its immediate surroundings at a high spectral resolution. Monitoring the spectral surroundings allows for better control of interferences and also enables simultaneous determination of multiple elements within the detection window.

This study presents a novel method for assessing environmental lead (Pb) contamination using HR-CS GF-AAS. The method enables the simultaneous determination of Pb alongside aluminum (Al) and iron (Fe). Al and Fe were chosen due to their minimal environmental mobility and serve to normalize Pb content for an assessment of lead contamination.

A high dynamic range was achieved by combining the use of spectral lines with different sensitivities and by measuring absorbance at multiple points within each spectral line. The method was developed for the analysis of Antarctic terrestrial flora, nonetheless, it is also generally applicable to environmental research studies involving various sample types.

SPECIATION OF ARSENIC, ANTIMONY, GERMANIUM AND TELLURIUM IN DRINKING WATER RESERVOIRS OVER THE SEASONS OF THE YEAR

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Current knowledge about cycling of elements and their species in natural environment is proportional to how challenging it is to obtain reliable analytical data. Two Czech reservoirs of contrasting chemistry and hydrological regime used as drinking water sources were chosen as study sites for observing changes of speciation of As, Sb, Ge and Te throughout the year. Vrchlice in Central Bohemia is a eutrophic lake, which becomes anoxic in summer, while oligotrophic or mesotrophic Souš in the mountainous area in North Bohemia remains well oxygenated throughout a year. From both reservoirs, samples from depth profile were taken in monthly intervals over the course of a year and fully characterized as to their physical and chemical properties.

Simultaneous analysis of species of germanium, arsenic and antimony was performed by hydride generation (HG)- cryotrapping (CT) and ICP MS/MS detection. Te speciation was analyzed separately by selective HG- ICP-MS/MS and total As and Sb concentrations were determined by ICP-MS/MS. Details of the methods and analytical challenges of analyses at (sub) ng/L concentration levels will be presented.

The results reveal very different behavior of each element. Arsenic speciation is the most influenced by the biota, which causes major occurrence of iAs^{III} and methylated As species in the productivity period while the presence of these species declines in winter. Also, iGe shows nutrient profile controlled by biogenic uptake: scavenging and partial regeneration from the sediments. In contrast, presence of methylated species of Ge and Sb is rather conservative throughout the year with near vertical depth profiles, and iSb^{III} was not found in the samples. For the first time, there are available systematic data on $Te^{IV/VI}$ speciation.

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MÖSSBAUER SPECTROSCOPIC INSIGHT INTO EFFECT OF MAGNETISM ON LATTICE VIBRATIONS

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Standard theory (ST) of the electron-phonon interaction (EPI) predicts that the effect of magnetism on EPI 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 showed that the impact of the EPI on the spin susceptibility of metals can be enhanced by two orders of magnitude in the case of itinerant magnetism [1]. In other words, the effect of the EPI on magnetic properties of metallic systems, and *vice versa*, is much more strong than commonly believed. Based either on calculations and/or on measurements some authors recently reported results that are at variance with the ST-predictions. In particular, M. S. Lucas et al. wrote [2]: “*The phonon densities of states of bcc Fe-V alloys across the full composition range were studied by inelastic neutron scattering, nuclear resonant inelastic x-ray scattering, and ab initio calculations. Changes in the PDOS were revealed at crossing the Curie temperature*”, B. Alling et al. based on disordered local moments molecular dynamics calculations came to the conclusion that [3]: “*Lattice vibrations strongly affect the distribution of local magnetic moment in experimental evidence paramagnetic Fe*”, and I. S. Tupitsyn et al. communicated that [4]: “*This theory (ST) neglects the effect of magnetism on lattice dynamics and fails to explain enhancement of the critical temperature in phonon-mediated superconductors.*”

In this lecture I will present results acquired by means of ^{57}Fe Mössbauer spectroscopy (MS) on σ -phase Fe-Cr, Fe-V and Fe-Cr-Ni, λ -phase NbFe₂ and Fe-As compounds as well as with ^{119}Sn MS and Nuclear resonance inelastic X-ray scattering (NRIXS) on metallic Cr. The common feature of all these systems is delocalized (itinerant) magnetism. The results give clear evidence that the lattice dynamics in the magnetic state of the investigated samples is meaningfully different than the one in the paramagnetic state. The latter means that magnetism and lattice vibrations, at least in the studied systems, are mutually dependent. Details on the issue can be found elsewhere [5].

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NEW NUCLEAR RESONANCE BEAMLINE ID14 AT ESRF

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In the beginning of 2024 the Nuclear Resonance beamline at the ESRF was opened for users after upgrade and movement from the ID18 to the ID14 section. The upgrade was aimed on bringing new possibilities (“Nanoscope” and “Spectrograph”) as well as make already existing techniques more stable (improved optics, temperature stabilization, etc.). The main aim of the new “Nanoscope” (specially designed KB mirrors) is to reach better spatial resolution, while “Spectrograph” will allow extreme energy resolution (down to ~ 50 μeV). Existing techniques such as synchrotron Mossbauer source (SMS), nuclear forward scattering (NFS), nuclear inelastic scattering (NIS) and others got the integral (over time) flux gain.

Now the beamline has temperature stabilization of two hutches. One with the “Nanoscope” to prevent movement of sample due to temperature expansion of the sample stage. Second stabilized hutch contains optics system (high-resolution monochromator, nuclear Bragg monochromator, spectrograph, etc.). It results in significantly improved stability of the beam flux. Thus, before at ID18 an adjustment of beamline optics was required every hour, but now at ID14 if the temperature stabilized hutch remain intact, the beam flux could be stable for at least three days. This leads to an increase in the integral flow by more than 25%, and makes *operando* and *in-situ* experiments more feasible due to the absence of adjustment pauses.

The new high-heat-load monochromator (HHLM) have a horizontal scattering plane. It was necessary to achieve a better beam quality in the vertical plane in which further optics (high-resolution monochromators, deflectors, etc.) work. Thus, canceling the heat-load effects in the vertical plane results in better stability and a smaller beam vertical size while using KB mirrors or “Nanoscope”.

The “Nanoscope” along with Extremely Brilliant Source (EBS) of the ESRF and new HHLM allows to reach an extreme spatial resolution, for example ~ 500 nm using SMS or ~ 150 nm with NFS. Even losing a part of intensity due to the smaller reflectivity of the “Nanoscope” compare to common KB mirrors, it still allows to increase the flux area density by factor of ~ 10 or more. The “Nanoscope” opens a new era of synchrotron Mossbauer techniques applications, almost 30% of new proposals already refer to it.

DEVELOPMENT OF TIN OXIDE PARTICLES DISTRIBUTED PHOSPHOVANADATE GLASS AS A CATHODE FOR SECONDARY BATTERY WITH HIGH PERFORMANCES

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Vanadate glass, having semiconductor-level electrical conductivity, is a promising candidate for a new cathode material for secondary batteries. This study investigated the relationship between the structure and cathode active performances of $x\text{P}_2\text{O}_5 \cdot (90-x)\text{V}_2\text{O}_5 \cdot 10\text{SnO}_2$ ($x\text{PVS}$) glasses with x from 10 to 60 mol%. The series of glass samples were prepared by melt-quenching and characterized by Differential thermal analysis (DTA), X-ray diffractometry (XRD), ^{119}Sn Mössbauer spectroscopy (SnMS), Electrochemical Impedance Spectroscopy (EIS), X-ray absorption fine structure (XAFS) and charge-discharge capacity test on lithium-ion batteries (LIB) and sodium-ion batteries (SIB). The DTA curves of $x\text{PVS}$ showed that the glass transition temperature (T_g) gradually increased from 256 to 622 °C with x from 10 to 60 mol%. This result indicates that the thermal durability of $x\text{PVS}$ increased with P_2O_5 content. In addition to halo XRD patterns attributed to the amorphous structure of $x\text{PVS}$, sharp and intense peaks due to SnO_2 were detected for $x\text{PVS}$ with x of 10 and 20. In contrast, the samples with x from 30 to 60 mol% showed the presence of SnP_2O_7 . Due to $\text{Sn}^{\text{IV}}\text{O}_2$, isomer shift (IS) of $-0.018_{\pm 0.001}$ mm s⁻¹ and quadrupole splitting (QS) of $0.520_{\pm 0.002}$ mm s⁻¹ were obtained from SnMS of 10PVS, while Sn^{IV} in SnP_2O_7 with IS of $-0.415_{\pm 0.001}$ mm s⁻¹ and QS of $0.332_{\pm 0.003}$ mm s⁻¹ were detected from SnMS of 60PVS. DC conductivity shows a monotonic trend and decreases from $\sim 10^{-5}$ (Ω cm)⁻¹ to $\sim 10^{-10}$ (Ω cm)⁻¹ at RT as V_2O_5 is gradually replaced by P_2O_5 . As of the result of the secondary battery performance test, the largest initial discharge capacities of 349 mAh g⁻¹ in LIB and 64.3 mAh g⁻¹ in SIB under the current density of 50 mA g⁻¹ were recorded using 10PVS cathode. As for the capacity retention in LIB, 10PVS was the highest at 71.5 %, while that for SIB was 67.3 %. In terms of the large capacity and capacity retention, it is concluded that 10PVS is the best cathode for secondary batteries among the investigated samples in this study.

119-SN MÖSSBAUER SPECTROMETRY USED IN THE STUDY OF TIN-CONTAINING METALLIC GLASSES

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119-Sn Mössbauer spectrometry is a less commonly used method than its 57-Fe counterpart. However, using both these methods allows us to obtain a more complete picture about the local atomic arrangement of Iron and Tin within the alloys that contain these elements as a part of their composition.

Hyperfine interactions in Fe₈₁B₁₂Sn₇ and (Fe₃Co₁)₈₁B₁₂Sn₇ metallic glasses were explored through ⁵⁷Fe and ¹¹⁹Sn Mössbauer spectrometry. As-quenched specimens were fabricated via planar flow casting, followed by annealing at 673 K for 30 minutes. This temperature coincides with a phase transformation in the studied systems as determined by differential scanning calorimetry measurements. Mössbauer spectrometry investigations at varying temperatures and in the presence of external magnetic fields probed hyperfine interactions between ⁵⁷Fe as well as ¹¹⁹Sn resonant nuclei and their electron shells. The effects of substitution of a quarter of Iron atoms by Cobalt are also discussed.

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MÖSSBAUER STUDY OF PLATINUM-DECORATED IRON OXIDE POWDERS DEVELOPED FOR GAS SENSING APPLICATIONS

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Protection against undesired concentrations of toxic, flammable or otherwise harmful gases accumulating in industrial or domestic environments requires the application of reliable gas sensors [1]. Various semiconductor metal oxides (such as SnO₂, α -Fe₂O₃) have been shown to be suitable candidates for the development of resistive gas sensors [1,2]. Additives, e.g., of noble metals, may be used to improve gas sensing properties of metal oxide based sensors under specific working conditions. With the aim to obtain a gas sensor material for hydrogen, we synthesized powders of α -Fe₂O₃ and Fe₃O₄ particles with nanotube morphology. Platinum with different relative concentrations was subsequently dispersed on the surface of the particles in order to facilitate selectivity for hydrogen. X-ray diffractometry and scanning electron microscopy were used to assess the structure and morphology of the samples. ⁵⁷Fe Mössbauer spectroscopy and X-band electron paramagnetic resonance spectroscopy measurements were performed on the samples at several temperatures. The resulted ⁵⁷Fe Mössbauer spectra revealed the presence of multiple magnetic components whose origin is going to be discussed.

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MÖSSBAUER STUDIES OF β -HEMATIN CRYSTALS: BRIDGING GAPS IN MALARIA RESEARCH

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Understanding the physical characteristics of the hemozoin crystal, and its synthetic version, the β -hematin, is very important for the design of antimalarials and for diagnosis of malarial disease [1,2]. In a previous work, we reported some physical characteristics of β -hematins synthesized from hemin in aqueous-acetate medium and in presence of varying concentrations of chloroquine [3]. It was proposed that the shapes of the experimental kinetics curves for β -hematin crystallization can be explained due to hemin dimer availability and to nucleation and growth. The β -hematins showed needle-like morphologies of 0,76 μm long and 0,14 μm wide. The presence of chloroquine affected their morphological characteristics by promoting crystal twinning formation, and crystals with lower sizes and with symmetrically tapered ends. We also found small variations in the relative intensities as well as in the relative peak broadenings in some of the X-ray Bragg reflections with increasing chloroquine concentration. The positions and intensities of the main IR absorption bands did not appreciably change with chloroquine concentration. In this work, we present the Mössbauer spectral characteristics of β -hematin crystals synthesized from hemin in two different reactive mediums and in the presence of two antimalarials. The 300 K and 10 K Mössbauer spectra of all samples were fitted with one or two asymmetric doublets using the Blume-Tjon model [4]. The asymmetric spectral components are ascribed to relaxation phenomena of the iron ions of the centrosymmetric dimers. The more asymmetric-like component suggests longer iron-iron distances, while the symmetric-like component can be ascribed to closer iron-iron distances. Mössbauer spectroscopy suggested that the spectral characteristics exhibited by the β -hematin crystals depended upon temperature, reactive medium, type of antimalarial and its concentration.


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MÖSSBAUER SPECTROSCOPY ANALYSIS OF FUNGAL-INDUCED STRUCTURAL CHANGES IN OCHRES

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Mineralogically diverse phases of (hydrated) ferric oxide-hydroxides can precipitate from the acid mine drainage at abandoned mine adits. These phases, commonly referred to as ochres, play a significant role in the immobilization of various potentially hazardous migrating elements in mine effluents, e.g. arsenic and antimony. In sediments, however, ochres interact with microorganisms, including the microscopic filamentous fungi, which induce biotransformation of mineral phases and their mixtures, arising from acid mine effluents, and thus can contribute to the mobilization of both essential and hazardous elements in the environment [1].

Structural changes in ochres and the consequences of these changes on the mobility and bioavailability of hazardous substances were determined during their incubation with microscopic fungi. In doing so, various spectral methods including X-ray diffraction, flame atomic absorption spectrometry, neutron activation analysis, and Mössbauer spectroscopy were applied. Natural Fe-containing ochres were collected at an abandoned antimony deposit in Pezinok, Slovakia.

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BIO- AND CHEMICAL APPLICATIONS OF MÖSSBAUER SPECTROSCOPY

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Iron is one of the most abundant elements on Earth and also in the applications of Mössbauer spectrometry. The present study is a summary of search for iron compounds in nano- and bulk materials that now play an important role in the development of specific areas of chemistry of iron, biological applications, pigments for various types of artworks and industrial applications.

The aim was to study iron-containing nanoparticles in different forms of materials; e.g. disks, powders, tissues, thin films, etc. The methods of preparation of nanomaterials have attracted considerable scientific interest in recent years. These materials are structurally well ordered and very well-defined and exhibit unique physical and/or chemical properties which determine their possible practical applications. The aim of the lecture is to give an overview of current trends and perspectives in the research of the above mentioned classes of nanomaterials.

Using Mössbauer spectrometry, different catalytic, biologically active systems and disks from steels were studied including temperature dependencies of selected biological tissues and synthetic vivianite. Mössbauer spectrometry was chosen as a principal method of investigation. Complex behaviour of magnetic and non-magnetic phases of nanomaterials was identified in the investigated samples by Conversion Electron Mössbauer Spectrometry and transmission technique. Their chemical composition was checked by neutron activation analysis and X-ray fluorescence. Structural arrangement was studied by scanning electron microscopy with energy dispersive spectrometry and transmission electron microscopy. In the presentation, I will discuss the properties of different types of nanomaterials intended for various applications.

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HOW MANY IRON COMPOUNDS ARE IN PHARMACEUTICALS CONTAINING FERROUS BISGLYCINATE CHELATE? STUDY USING MÖSSBAUER SPECTROSCOPY

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Ferrous bisglycinate chelate (C₄H₈FeN₂O₄) is used for some antianemic pharmaceuticals. This chelate registered as Ferrochel® was announced as a most stable compound [1]. The first study of pharmaceutical product with Ferrochel® by Mössbauer spectroscopy showed the presence of ~60% of ferric compound [2]. Recently a new series of iron-containing pharmaceutical products was studied by XRD, magnetization measurements and Mössbauer spectroscopy [3]. The strangest results were obtained for the products from different manufacturers containing ferrous bisglycinate chelates. Therefore, in this work we compare three pharmaceutical products containing ferrous bisglycinate chelates, namely: Gentle Iron, Hema-Plex® and Iron Bisglycinate. The Mössbauer spectra showed the presence of 9 ferrous and 2 ferric, 4 ferrous and 3 ferric, and 7 ferrous and 3 ferric compounds, respectively in these products. Moreover, both the spectra of Gentle Iron and Hema-Plex® additionally contained two magnetic sextets corresponding to α-Fe and an unknown compound.

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IS THERE SOMETHING REALLY NEW IN THE FIELD OF MATERIALS ANALYSIS? SPOILER: YES, THERE IS.

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Laboratory X-ray source based high-energy-resolution spectrometers have been showing a renaissance that culminated in radical progression recently. Although techniques like X-ray Absorption Near Edge Structure (XANES), Extended X-ray Absorption Fine Structure (EXAFS) or X-ray Emission Spectroscopy (XES) were pioneered mainly on laboratory scale instruments, they have matured dramatically with the advent of synchrotron X-ray sources. The obvious excellence of these large scale photon sources in terms of X-ray brilliance, energy tunability, polarization, pulsed time structure, etc. over the conventional X-ray tubes turned the techniques mentioned dependent almost exclusively on occasionally accessible synchrotron beamtimes. However, the emergence of modern laboratory X-ray tube based spectrometers in the recent decade is being widely recognised, which give rise to a clear demand for such instruments.

Here, a short overview will be given on the present status of lab-based high-energy-resolution X-ray spectrometers with selected use cases.

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MÖSSBAUER ANALYSIS OF THE GOETHITE AND HEMATITE CONTENT OF PALEOSOLS AND GOETHITE NODULES FROM THE CARPATHIAN BASIN REGION

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Goethite and hematite are typical iron minerals in various primary iron ores and sediments. Their formation is closely related, ranging from hydrothermal to microbial processes. The provenance of the goethite and hematite fraction of a given sample strongly depends on the geological history of the site where it is found. The grain size distribution of the minerals is closely related to their origin as well as to possible eolian or fluvial transport, and it is of crucial importance for the formation of soils. Such data on possible paleosols are helpful to estimate climate changes in a given region, including temperature and precipitation characteristics.

In the case of bulk samples and when other constituent minerals do not hinder the detection of diffraction lines, XRD is a good tool for identifying goethite and hematite. Quantitative determination is a more significant challenge with the XDB method especially when the overlap of the diffraction lines is substantial.

For a quantitative and qualitative analysis, ⁵⁷Fe-Mössbauer Spectroscopy, with its ideal selectivity for iron-containing phases, is a useful tool even when the too-low particle size makes XRD useless.

Since the decrease of the particle size (below 10-12 nm in diameter) results in superparamagnetism, the Mössbauer spectra can show up in a different way, presenting paramagnetic doublets instead of structure-rich magnetically split patterns. The magnetic splitting also depends on the temperature of the measurement and on the possible impurities (e.g., Al) in the goethite or hematite phase.

These features of the Mössbauer analysis can help the determination of the goethite and hematite content of the investigated sample while providing additional information on the particle size distribution and possible impurities. On the basis of a large number of samples collected in the Carpathian basin, we demonstrate under what experimental condition it is recommended to achieve reliable qualitative and quantitative Mössbauer analysis for goethite and hematite.

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QUANTITATIVE ANALYSIS IN MÖSSBAUER SPECTROSCOPY

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Despite Mössbauer spectroscopy being frequently applied in materials science, its utilization in industry remains rather limited, even though Mössbauer techniques offer several advantages compared to other analytical methods. One important industry segment, where Mössbauer spectroscopy can be beneficial, is steel production and metallurgy, as it can provide crucial information for validation and quality control of the steel production process. The determination of retained austenite in steels is a key issue in this sector including the crucial task of the ratio of individual phases (volume or mass) within the steels.

Metallography and X-ray diffraction are commonly employed for this purpose, given their already established standardization. However, Mössbauer-based techniques offer several advantages over these methods; nevertheless, they are yet to be standardized.

This work discusses the most important issues connected with the determination of individual quantities using transmission Mössbauer spectroscopy, conversion X-ray Mössbauer spectroscopy, and transmission Mössbauer spectroscopy with a resonant detector, in comparison with X-ray diffraction.

As no standard material for the quantitative determination of retained austenite exists, this research focuses on a model system of two powders mixed in precise ratios, namely hematite exhibiting a sextet spectrum and zinc ferrite exhibiting a doublet with low quadrupole splitting (the two lines still significantly overlap). A set of mixtures with mass ratios of the two materials (nominal ratio of hematite ranging from 0 to 1) was prepared by homogenizing in a ball mill and measured using transmission Mössbauer spectroscopy [1], conversion X-ray Mössbauer spectroscopy [2], and transmission Mössbauer spectroscopy with a resonant detector and X-ray diffraction, and the hematite/zinc ferrite ratio was determined. The obtained results are discussed in detail.

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ELECTRODEPOSITION OF ^{57}Fe IRON THIN FILMS ON PIEZOFILMS FOR MÖSSBAUER GAMMA OPTICS

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Mössbauer spectroscopy finds applications in various research domains, such as materials science, physics, chemistry, and biology. Recently, it has been applied in the rapidly developing field of nuclear quantum optics, where electronically induced transparency (EIT) and acoustically induced transparency (AIT) are used for gamma photon manipulation [1]. This involves generating trains of short gamma photon pulses, for instance, through ultrasonic vibration of resonant absorbers [2]. However, constructing gamma optical elements is a challenging task, and their properties significantly impact gamma photon manipulation efficiency. Iron foils are traditionally glued to gamma-transparent piezoelectric elements like PVDF. However, this method has issues with repeatability, increased photon absorption from the glue, and potential deterioration of ultrasonic vibration homogeneity.

This study presents an alternative approach for depositing thin ^{57}Fe films onto the piezoelectric foils using electrodeposition. Unlike other techniques such as sputter coating, this process enables the creation of thicker films with predetermined thickness while minimizing initial material requirements and losses. The procedure involves several steps: sputter coating of a thin conductive film onto the piezo element, electrodeposition of a thin film from ^{57}Fe electrolyte solution, washing and coating. The deposited layers were then characterized through Mössbauer spectroscopy, mass spectroscopy, X-ray diffraction, light microscopy, and scanning electron microscopy.

The plastic piezo was coated with approximately 3 μm thick layers of ^{57}Fe α -iron, with minor impurities of amorphous iron oxides. The prepared elements demonstrated sufficiently homogeneous movement, making them suitable for gamma optics experiments. Furthermore, these components may serve as effective calibration tools for Mössbauer spectrometers across a broad energy range ± 15 mm/s, offering over 18 calibration points and enabling precise determination of Doppler modulation linearity.

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COMPARISON OF SCINTILLATION AND SEMICONDUCTOR DETECTORS IN MÖSSBAUER SPECTROSCOPY

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Mössbauer measurements may require anywhere from several hours to possibly several days or weeks to acquire sufficient statistics. Detector properties, such as efficiency, energy selectivity, dark counts, and detection of unwanted radiation, greatly influence the spectra accumulation time. Among the most employed detectors are gas proportional detectors, scintillation detectors, and increasingly popular semiconductor detectors. Through careful selection of the detector, one could potentially save a considerable amount of time. This work focuses on comparing scintillation and semiconductor detectors and evaluating the amount of time saved by employing one detector over the other.

Semiconductor detectors typically offer outstanding energy resolution and produce short induced pulses (nanoseconds). On the other hand, scintillation detectors then excel at gamma photon detection efficiency and the ability to utilize large active areas. However, they suffer from lower energy resolution, and higher decay time.

The work focuses on comparing an Yttrium Aluminum Perovskite doped with Cerium (YAP:Ce) scintillation detector with a silicon semiconductor detector. We compare several important parameters, most notably the signal-to-noise ratio (SNR) of measurements on multiple samples encompassing all different variants of Mossbauer samples. Those are samples with high electron and high nuclear absorption (α calibration iron), low electron and high nuclear absorption (enriched iron hexacyanide - $\text{K}_2\text{MgFe}(\text{CN})_6$), low electron and low nuclear absorption (thin non-enriched iron hexacyanide) and high electron and low nuclear absorption (thick sample of non-enriched iron hexacyanide). All the samples were measured in transmission Mössbauer geometry. Finally, we quantified the time reduction to attain equivalent SNR levels when employing the semiconductor detector.

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CONTROLLING THE PROPERTIES OF NANOSIZED CoFe_2O_4 PREPARED WITH THE HYDROTHERMAL SYNTHESIS

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The hydrothermal one-pot synthesis allows the preparation on nanosized metal oxides particles with high yields of reaction. Additionally, the use of water as a solvent avoids the use of potentially hazardous chemicals that are usually associated with other methods (thermal decompositions in high-boiling solvents). In this study, we present the preparation and characterization of nano- CoFe_2O_4 of different sizes and a high degree of monodispersity. The size of the nanoparticles could be controlled by altering the time of reaction. The samples characteristics were studied with several techniques: the transmission electron microscopy (TEM), gas adsorption, vibrating sample magnetometry (VSM), X-ray powder diffraction (XRD) and Mössbauer spectroscopy (MS). The detailed exploration of samples' characteristics allows to assess the performance in the selected application with the respect to the physicochemical properties. The selected samples were tested in the dye degradation experiments [1,2].

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50 YEARS OF SURFACE-ENHANCED RAMAN SPECTROSCOPY: FROM FUNDAMENTALS TO INNOVATIVE APPLICATIONS

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Surface-enhanced Raman spectroscopy (SERS) was discovered by Fleischmann et al. who reported in 1974 a strong enhancement of the Raman scattering of pyridine on an electrochemically roughened silver electrode [1]. This discovery led to intense theoretical research on the origin of Raman enhancement. On the other hand, because of many experimental problems, the SERS remained a technique studied by a limited number of research groups. The first report about single-molecule (SM) detection by SERS (SM-SERS) in 1997, the first experimental evidence of TERS in 2000, and, in particular, the intense development of nanotechnologies (notably in terms of SERS enhancing substrate design and functionalization) dramatically extended the field of SERS research and applications [2].

Nowadays, SERS is understood as a technique providing an enormous enhancement (10^4 – 10^{11}) of the Raman signal of molecules adsorbed on suitable metallic or semiconductor nanostructural surfaces [3]. 50 years after its discovery, SERS has become a fully grown spectroscopic technique with a rapidly expanding number of applications in the chemical, material, and particularly life sciences [2,3].

In this talk, I will summarize the basic theoretical and experimental aspects, innovative applications, and further prospects of the SERS technique. I will also highlight the contribution of the strong “Czech SERS group” represented by Prof. B. Vlčková and a number of her former students.

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EXPLORING THE SYNERGY OF ELECTROCHEMISTRY AND SURFACE-ENHANCED RAMAN SCATTERING (EC-SERS) FOR ADVANCED SURFACE ANALYSIS

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Surface-enhanced Raman scattering (SERS) spectrometry is indeed a potent tool in physico-chemical and analytical research, particularly for its ability to detect trace amounts of compounds adsorbed on specialized plasmonic sensors. Despite its decades-long existence, SERS continually reveals new insights into surface phenomena. The enhancement of the Raman signal in SERS is influenced by numerous factors, including the type of metal used, sensor morphology, analyte concentration, excitation energy, irradiation time[1], temperature, and last but not least, the electrochemical potential applied to the sensors. Such surface modification, related mostly to the Fermi-level of metal or surface charge, can induce some of enhancement mechanisms or significantly impact the type of adsorption.

The integration of electrochemistry and SERS, referred to as EC-SERS, offers a unique perspective on this technique. EC-SERS enables the acceleration of molecule adsorption, control over the adsorption/desorption processes[2-3], exploration of diverse adsorption mechanisms[4], *in-situ* investigation of surface reactions[5], and more. This combination facilitates a deeper understanding of surface interactions and opens avenues for innovative applications in various fields, including chemistry, material science, and biochemistry.

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THE ROLE OF ADSORPTION SITES ON Ag NANOPARTICLE SURFACES IN SERS SPECTROSCOPY AND PLASMON CATALYSIS

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Surface-enhanced Raman scattering (SERS) spectroscopy is currently a well known spectroanalytical method. Recently, it has been established also as an excellent tool for monitoring plasmon-catalyzed reactions undergone by molecules adsorbed on plasmonic metal nanostructured surfaces upon irradiation. While the principal electromagnetic mechanism of SERS is dependent entirely on the characteristics of the plasmonic metal nanostructured surface, operation of the molecular resonance mechanism (in SERRS and/or the chemical mechanism of SERS) is strongly dependent on the surface-adsorbate interaction. Our comparative studies [1,2] have demonstrated that in the case of Ag nanoparticle surfaces, this interaction is principally influenced by the oxidation state of Ag adsorption sites. In particular, 2,2'-bipyridine (bpy) has been established as a reliable SERS spectral probe for this purpose. In the presence of entirely the oxidized Ag^+ adsorption sites, Ag^+ -bpy surface species has been detected, while after modification of Ag NP surface by chlorides and/or upon a reduction-driven Ag NP growth in the presence of bpy, formation of a new Ag(0)-bpy surface complex has been established with help of factor analysis [2]. Importantly, SERS excitation profiles of the Ag(0)-bpy bands have revealed a photoinduced charge transition with a maximum at ca 540 nm, while no such effect was observed for the Ag^+ -bpy species [1]. Recently, plasmon-catalyzed decarboxylation reactions of $\text{Ru}(\text{bpy})_2\text{dcbpy}$ and $\text{Ru}(\text{dcbpy})_3$ ($\text{dcbpy}=4,4'$ -dicarboxybipyridine) complexes on Ag NP surfaces have been revealed to proceed entirely under the conditions for which the presence of Ag(0) adsorption sites was established earlier by the bpy spectral probe [3]. The presence of Ag(0) adsorption sites as the necessary condition of the reaction progress is in full accord with the charge carriers /namely hot electrons (e^-) and hot holes (h^+)/ mechanism of plasmon catalysis. In particular, the neutral Ag(0) sites create the interface required for the transport of hot e^- to H^+ co-reactants complementing thus the C-C bond breaking and CO_2 formation caused by hot h^+ [3].

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INTERFEROMETRIC SCATTERING MICROSCOPY REVEALING HOTSPOT DYNAMICS DURING FLUCTUATIONS IN SINGLE MOLECULE RAMAN SPECTROSCOPY

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Surface-enhanced Raman scattering (SERS) exhibits pronounced intensity fluctuations at the single molecule regime, spanning a wide range of timescales, with events as rapid as tens of microseconds [1]. For reaching a single-molecular level of sensitivity, an overall enhancement of at least 10^7 is required, which is typically achievable in a nm-sized gaps between plasmonic nanoparticles [2]. Maximal enhancement and resonant wavelength of these so called ‘hotspots’ is highly dependant on the exact gap size [3]. Given that SERS signal is highly dependant on the hotspot arrangement, monitoring hotspot dynamics is crucial to elucidate the origin of the signal fluctuations. To investigate the impact of substrate dynamics in a liquid environment, interferometric scattering microscopy (iSCAT) emerges as a valuable tool. iSCAT not only enables the localization and characterization of substrates as diminutive as 2 nm with high spatial and temporal resolution but also facilitates the assessment of polarization effects [4]. Employing polarization-sensitive iSCAT optimizes enhancement based on nanoparticle orientation and allows for the determination of hotspot gap sizes.

Here we present concurrent measurements of polarization-sensitive iSCAT and single-molecule SERS using excitation wavelengths of either 561 nm or 640 nm. We demonstrate the proficiency of iSCAT in characterizing the hotspot and its dynamics, especially in cases where only two 30 nm sized nanoparticles are involved, achieving a temporal resolution in hundreds of microseconds. Finally, we elucidate hotspot dynamics during high intensity fluctuations and their contribution across various scenarios.

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FEMTOSECOND STIMULATED RAMAN SPECTROSCOPY IN DECIPHERING SWITCHING MECHANISM OF BIOLOGICAL PHOTORECEPTORS

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Orange Carotenoid Protein (OCP) is a unique photoprotective, water-soluble protein predominantly found in cyanobacteria [1]. It plays a critical role in non-photochemical quenching (NPQ), a protective process that dissipates excess absorbed light energy as heat, safeguarding photosynthetic organisms from photodamage. The vibrational characteristics of optically excited echinenone in various solvents and the Orange Carotenoid Protein (OCP) in red and orange states were systematically investigated through steady-state and time-resolved spectroscopy techniques. Time-resolved experiments, employing both Transient Absorption (TA) and Femtosecond Stimulated Raman Spectroscopy (FSRS), reveal distinctive components corresponding to different states in the OCP photoactivation process. The time-resolved studies indicate more defined vibrational signatures during the initial 140 fs of carotenoid evolution in OCP, an absence of a clear vibrational signature for the relaxed S1 state of echinenone in OCP, and more robust signatures of a highly excited ground state (GS) in OCP. Differences in S1 state vibration population signatures between OCP and solvents are attributed to distinct conformations of echinenone in OCP and hydrogen bonds at the keto group forming a short-lived intramolecular charge transfer state. The vibrational dynamics of the hot-GS in OCP show a more pronounced upshift compared to echinenone in solvents, thus suggesting an unusually hot form of GS. The study proposes a hypothesis for the photoactivation mechanism of OCP, emphasizing the extraordinarily high level of excitation in longitudinal stretching modes as a driving force. The study underscores the importance of vibrational analysis in understanding the intricate processes involved in OCP photoactivation.

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NOBLE METAL NANOSTRUCTURES USED IN SPECTROSCOPIES

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Engineered noble metal nanostructures have been developed and investigated in our laboratory for some time already. Our attention is mainly focused on (a) nanoparticles used in surface-enhanced Raman scattering (SERS) spectroscopic detection of selected (bio)molecules [1, 2] and (b) nanoclusters employed as luminescent centers within functional nanocomposites [3-6]. From a particular viewpoint, nanometer scale is quite large, hence, there is no wonder that nanostructures manifesting themselves by sizes of dozens of nanometers and/or units of hundreds of nanometers (so called nanoparticles) have completely different features than the same type of material confined into 0.2-2 nm (i.e., nanoclusters). Characteristic surface plasmon extinction (SPE) of noble metal nanoparticles is frequently exploited in SERS spectroscopy, while noble metal nanoclusters possessing intrinsic fluorescent properties can be efficiently used in sensing and bio-imaging. In our contribution, we would like to show our very recent achievements in nanoparticle and nanocluster size domains as well as will try to envisage our future research.

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DROPLET DEPOSITION RAMAN SPECTROSCOPY TECHNIQUES AND THEIR APPLICATIONS

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The droplet deposition Raman spectroscopy is based on the small drop deposition of analyte on a suitable (generally hydrophobic) solid surface. If the flow in a drying liquid sample carries dispersed material to the droplet edge, it forms coffee-ring or small spot patterns where the analyte is pre-concentrated [1,2]. This approach and its combination with surface-enhanced Raman spectroscopy (SERS) and graphene-enhanced Raman spectroscopy (GERS) have received considerable attention in the field of sensitive Raman detection using analyte pre-concentration. This contribution will summarize fundamentals, experimental aspects, and some advanced applications of mentioned techniques.

Two main advantages of droplet deposition Raman techniques are principally considered: the sensitivity of detection of various analytically important molecules and the drying-induced segregation of the components from the mixtures (such as body fluids). For example, recently, we reported that the spatial segregation of lipids and carbohydrates from pure infant formula into dried patterns was confirmed by Raman spectral mapping [3]. Lipids tended to accumulate in the coffee-ring, and carbohydrates formed the thin layer in the central part of the ring. The same separation in the dried pattern was also observed for melamine-blended infant formula, where melamine was detected only from the thin central layer together with carbohydrates due to the melamine glycation by lactose. Therefore, we could profit not only from the efficient pre-concentration and drying-induced spatial separation but also from the chemical reaction potential of molecules of interest present in a complex solution or suspension.

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RAMAN MICROSCOPY OF CELLS AND TISSUES: FROM CRYSTALLINE INCLUSIONS TO VIRAL FACTORIES

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In recent decades, Raman microscopy has been gaining ground in biological, biophysical, and biomedical research. Its advantages are molecular specificity, non-contact and non-destructive character, and simple sample preparation. Thanks to technical and methodological progress, Raman imaging based on chemical contrast enables the study of the molecular composition of intracellular structures in unicellular organisms as well as the monitoring of some processes in cellular tissues. In this contribution, we use selected examples to demonstrate how Raman microscopy has contributed to the elucidation of the chemical composition of crystalline structures of eukaryotic microorganisms, especially but not exclusively purine crystals in protists and photosynthetic microalgae [1-3]. Furthermore, we will show how Raman microscopy can be useful in studying the processes behind viral infection by complementing the information provided by electron microscopy, time-resolved fluorescence, and holotomography microscopy [4]. We will show that despite certain limitations and difficulties, confocal Raman microscopy can provide an important piece of the puzzle allowing a deeper understanding of various biological phenomena and processes.

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CRYOMAGNETIC SPECTROSCOPIES ON VAN DER WAALS MATERIALS USING CHIRAL LIGHT

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Van der Waals materials and their heterostructures exhibit remarkable electronic and optical properties that can be finely tuned using external physical fields such as photonic, magnetic, electric, and strain, or through proximity effects with other materials and molecules. These attributes position them as superior building blocks for cutting-edge optoelectronic and spintronic devices. Raman (Ra) and photoluminescence (PL) micro-spectroscopies stand out as pivotal tools for delving into the electronic, optical, and spin phenomena within two-dimensional materials (2DMs) and their heterostructures [1-3]. Leveraging light with intrinsic chirality, these spectroscopic techniques offer a window into spin and valley-driven physics across diverse 2DMs. Of particular significance, Ra and PL spectroscopies facilitate the exploration of magnetic order and quantum phenomena in van der Waals materials, owing to the robust spin-lattice coupling [4]. Notably, recent advancements have unveiled the potential of the Ra/PL microscopy in elucidating magnetization reversal and magnetic domain mapping in various 2D magnets and their heterostructures under applied magnetic fields. In this presentation, I will showcase selected findings from helicity-resolved cryomagnetic spectro-microscopies conducted on prominent 2DMs, shedding light on their intriguing properties and potential applications.

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COMBINED VIBRATIONAL SPECTROSCOPIC AND STRUCTURAL STUDY OF MOLECULAR NLO MATERIALS

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Nowadays, a part of materials research is focused on the search for new molecular crystals for nonlinear optics (NLO) based on organic polarizable molecules, their salts and co-crystals. NLO materials can be used in a wide range of technical applications that take advantage of numerous NLO effects (including SHG - Second Harmonic Generation, THG - Third Harmonic Generation, and cascaded self-frequency doubling and tripling), most notably in the generation of new laser frequencies, signal processing, optical communications, all-optical switching, optical power limiting and image manipulation.

The resulting molecular materials benefit from the presence of hydrogen bonding as a key interaction in the molecular self-assembly process leading to crystal formation. The energy of the hydrogen bonds formed counteracts the natural tendency of organic molecules to form centrosymmetric pairs, which is excluding $\chi^{(2)}$ processes.

This contribution presents the study of selected hydrogen-bonded molecular materials - e.g. salts of guanidine, pyrimidine and their amino derivatives with selected inorganic/organic anions - by the combination of experimental (IR spectroscopy, Raman spectroscopy, X-ray diffraction and calorimetry) and theoretical (solid state quantum chemical calculations) methods. The application of vibrational spectroscopy stems from the exceptional usefulness of IR and Raman spectroscopy for phase analysis and the study of phase transformations. In addition, the detailed assignment of the spectra allows the understanding of the vibrational contributions to hyperpolarizability and the processes associated with Stimulated Raman Scattering (SRS) [1, 2].

Last but not least, the linear and nonlinear optical properties of the studied materials will be presented and discussed

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APPLICATION OF RAMAN SPECTROSCOPY IN THE STUDIES OF 2D MATERIALS

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Raman spectroscopy is a very important tool enabling the characterization of 2D materials already since the discovery of graphene. In this case, Raman spectroscopy enabled the studies of defects, doping, and strain in this material. Furthermore, the application of this tool can be extended to the studies of functionalized graphene or other 2D materials. I will review our activities in this field with a particular focus on our recent achievements regarding the monitoring of graphene functionalization and the study of MoS₂ interactions with clean metallic surfaces in UHV conditions.

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CZECH AND SLOVAK SPECTROSCOPY INTERACTIONS - HISTORY AND FUTURE

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The foundations of Czechoslovak, Czech and Slovak spectroscopy were laid already in the 17th century, and in the course of the following period, important personalities appear on the scientific scene of both nations. We know the names of some of them in connection with important scientific discoveries of worldwide importance. Support for communication between Czech, Slovak and foreign scientists, researchers and experts has been provided by spectroscopic-themed conferences organized by spectroscopic societies from the middle of the twentieth century until the present day. Current congress activities take place on a bilateral basis, but also on the ground plan of the Visegrad Four countries and Germany. The research cooperation of our experts from the academic sphere as well as from routine or research laboratories in industry and other areas of practical use has long been carried out within and with the support of state institutions and grant agencies.

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LASER-BASED MID-IR ABSORPTION AND DISPERSION SPECTROSCOPY OF LIQUIDS

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When interacting with gaseous or liquid samples, laser radiation does more than attenuate light intensity; it also induces a phase shift in the transmitted light and heats the sample containing the analyte. While direct absorption spectroscopy primarily exploits intensity attenuation, these additional effects form the basis for dispersion spectroscopy and indirect methods like photoacoustic and photothermal spectroscopies.

This presentation will review potential measurement modalities, highlight recent instrumental advancements, and showcase selected applications. For liquid sensing, we employ broadly tunable external cavity quantum cascade lasers. We demonstrate their use in measuring protein secondary structures in water, exemplified by in-line detection in liquid chromatography [1] and protein melting experiments [2] as well as the use of lab-on-a-chip systems [3]. Dispersion spectroscopy will be introduced through measuring ethanol in water [4], illustrating its suitability for dynamic reaction monitoring. This will include observing the enzyme-catalyzed hydrolysis of sucrose into glucose and fructose [5].

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THERMOTROPIC PHASE TRANSITION OF DEHYDRATED PHOSPHOLIPIDS MONITORED BY DROP COATING DEPOSITION RAMAN (DCDR) SPECTROSCOPY

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Phospholipids are the major building blocks of cell membranes. To understand their unique properties and behavior under diverse conditions, liposomal suspension is commonly used as a model membrane system. One of the fundamental phospholipid properties is thermotropic mesomorphism. Upon heating phospholipid crystals undergo one or several intermediate phase transitions. The most prominent one, known as a main phase transition, is from a gel phase to a liquid crystalline phase. The transition temperature T_m at which the transition occurs is specific for different lipids. More techniques are currently available to monitor phase transitions including differential scanning calorimetry, nuclear magnetic resonance, fluorescence spectroscopy, or vibrational spectroscopy. Raman spectroscopy as a method providing unique information based on the vibrational motion of molecules appears to be particularly sensitive to lipid conformational changes present during the phase transition. Raman spectra obtained from the gel and liquid crystalline state of lipids directly reflect changes related to the structural alternations during the transition.

Here we focused on monitoring the main phase transition of selected phospholipids in a dried state employing drop coating deposition Raman (DCDR) spectroscopy. DCDR is based on the drying-induced pre-concentration of the studied analyte into the dried pattern (coffee-ring for lipids) from which the classical Raman spectra are acquired. Only a small volume ($\sim\mu\text{l}$) of low-concentrated ($\sim\text{mM} - \mu\text{M}$) sample is required [1,2]. Raman spectra from dried patterns of different phospholipids (differing in acyl chain length and type of the head group) were acquired in the temperature range covering their phase transition. Changes in spectral bands (intensity ratio, wavenumber shift) related to the phase transition were observed mainly in spectral regions for C-H stretching vibrations ($2800\text{--}3100\text{ cm}^{-1}$) or C-C stretching vibrations ($1050\text{--}1150\text{ cm}^{-1}$) of alkyl chains.

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EXPLORING CONFORMATIONAL CHANGES VIA SURFACE-ENHANCED RAMAN SPECTROSCOPY ASSISTED BY INTERFEROMETRIC SCATTERING MICROSCOPY

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Surface-Enhanced Raman Scattering (SERS) stands as a robust tool for exploring the behavior of diverse molecular species near plasmonic surfaces [1]. The nuanced spectral response of SERS is known to depend on the various experimental variables, including excitation wavelength, plasmonic metal, substrate morphology, and molecular orientation relative to the surface [2]. Despite the collective influence of these factors on SERS spectra, unraveling their united effects remains a formidable challenge. In parallel, Interferometric Scattering Microscopy (iSCAT) has emerged as a valuable instrument for exploring the dynamic behaviors of individual entities, such as proteins and nanoparticles, at nanometer scales with single molecule sensitivity [3,4]. iSCAT offers a unique vantage point on the interplay between molecules and enhancing substrates, enriching our understanding of surface-enhanced Raman probing.

This study showcases the unique fusion of these methodologies as a potent duo for tracking molecular conformational changes near plasmonic surfaces. While SERS excels in investigating of molecular structure and orientation, iSCAT enriches our insights from the substrate's perspective. Augmenting our analysis, we employ density functional theory (DFT) calculations to extract maximal information from our data. Utilizing gold nanoparticles (GNPs) coated with cysteamine as our model system, we unveil several structural alterations induced by cysteamine binding to the GNPs' surface, including torsion angle deformation. These modifications are distinctly reflected in the SERS spectra, evidenced by shifts in vibrational band positions.

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NANOPARTICLE COUNTING BY LASER-ASSISTED MASS SPECTROMETRY

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The detection of single microscopic entities has always posed a challenge. Laser-assisted mass spectrometry methods offer chemical information as well as imaging capabilities. Here, we demonstrate that mass spectrometry imaging can monitor individual gold and silver nanoparticles using two ionization techniques: laser ablation inductively coupled plasma (LA ICP)¹ and subatmospheric pressure laser desorption/ionization (LDI)^{2,3}. The principles allowing the detection of individual nanoparticles are explained, and the nanoparticle detection efficiency is discussed. The potential applications of the methods are demonstrated by detecting nanoparticles on biological tissues and imaging viable cells on 3D aggregates of human colorectal carcinoma cells.

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ARSEN, SELEN, TITAN ... SINGLEQUADEM SE NEDOMĚŘÍŠ

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This presentation provides a comparison of Thermo Scientific Single Quadrupole (SQ) and Triple Quadrupole (TQ) Inductively Coupled Plasma Mass Spectrometry (ICP-MS) techniques, with a focus on their applications for the detection and analysis of arsenic, selenium, and titanium. While SQ ICP-MS is a widely used and versatile tool in elemental analysis, it faces significant limitations when dealing with complex matrices and elements prone to polyatomic interferences, such as arsenic, selenium, and titanium.

TQ ICP-MS, on the other hand, offers advanced capabilities by incorporating an additional quadrupole mass filter and collision/reaction cell technology. This setup effectively mitigates interferences, enhancing detection limits and accuracy for these challenging elements. The presentation will explore case studies and empirical data demonstrating the superior performance of TQ ICP-MS in environments where SQ ICP-MS falls short. Key topics will include the mechanisms of interference reduction, the impact on analytical precision and accuracy, and practical considerations for implementing TQ ICP-MS in routine and specialized analyses.

This comparative analysis aims to underscore the critical advantages of Thermo Scientific TQ ICP-MS in the context of arsenic, selenium, and titanium detection, highlighting its essential role in achieving reliable and precise results in complex sample matrices.

NANOPARTICLES AS A NEW TOOL TO DIAGNOSE ISCHEMIC STROKE

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Ischemic stroke (IS) was identified as the second most common cause of death worldwide in 2019 according to a survey [1]. A significant percentage of patients remain with permanent consequences that can persist even fifteen years after the event [2]. This is also associated with economic impacts on healthcare and supportive services, which amounted to approximately 60 billion euros in the EU in 2017 [3]. The key to success is time. IS can already be precisely diagnosed nowadays. However, in each specific situation, there is a problem with detecting the onset of stroke, which is crucial for choosing the appropriate treatment and thus saving lives. Today's commonly used medical scanning devices can only visualize clots with high erythrocyte content. Other forms of thrombi become exceedingly difficult to recognize [4]. Polyiodinated biodegradable nanoparticles (IoNPs) have the potential to solve this problem. The current preliminary phase of research is focused on the distribution of elements in selected organs of laboratory animals. For the creation of an element distribution map, the unique method LA-ICP-MS is used in combination with μ CT 3D volumetry results of the brain. Results to date show the success of the functioning analysis method and nanoparticles detection in the laboratory rat's bloodstream, livers, and spleens. A new technique for radiocontrast staining using caesium was developed.

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CADMIUM ACCUMULATION IN ORGAN TISSUES AFTER INHALATION OF CADMIUM-BASED NANOPARTICLES

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Cadmium and its toxic effects are a very current issue at this time, as poisoning by this element can cause serious health problems or even death. Cadmium is transported through the bloodstream and is found in a wide range of tissues. Thus, long-termed exposure to cadmium can lead to cancer and adverse effects on organ systems (skeletal, reproductive, cardiovascular, etc.).^[1]

The distribution of cadmium and other biogenic elements was studied in the organs of mice - lungs, livers and kidneys. For the inhalation experiment, mice were divided into 3 groups. The first group was continuously exposed to CdO NPs for 6 and 9 weeks. The second group was exposed to CdO NPs for 6 weeks and then inhaled clean air for 3 weeks to determine whether the CdO NPs were permanently deposited in the tissues. In the third group (the control group), mice were exposed to the same conditions at each time point but breathed only clean air. After each exposure period, the mice were sacrificed and the organs were dry frozen, placed in agar medium, and cut into 20 µm thin cryosections. Organ cryosections were analyzed by laser ablation combined with inductively coupled plasma mass spectrometry using a Nd:YAG laser.

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A LITTLE JOURNEY FROM SINGLE DOMAIN PARTICLES TO SINGLE MOLECULE MAGNETS

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Superparamagnetic iron particles play an important role e.g. as magnetic drug carriers, in magnetic hyperthermia therapy and in heterogeneous catalysis. Already in the early days of the Mössbauer effect Mössbauer spectroscopy became an important tool to characterize iron phases in particle systems. Particle size determination via field dependent Mössbauer spectroscopy performed above the superparamagnetic blocking temperature was introduced by Mørup already in the 1980s [1]. Later, this method was also used for the identifications of metallic iron particles in the cavities of zeolites with having a size of only app. 100 atoms [2,3].

In this presentation, recent temperature and field dependent Mössbauer spectroscopic studies of even a smaller system with only 19 ferric high spin iron atoms showing ferrimagnetic order at LHe temperatures will be presented. This molecular nanodisc has the chemical formula $[\text{Fe}_{19}(\text{metheidi})_{10}(\text{OH})_{14}\text{O}_6(\text{H}_2\text{O})_{12}]\text{NO}_3 \cdot 24\text{H}_2\text{O}$ and displays single molecular magnetism with a 16 K anisotropy barrier [4]. To explore the vibrational modes of this nanodisc nuclear inelastic scattering (NIS) experiments have been performed and the so determined partial phonon density of states (pDOS) has been simulated using density functional theory (DFT) calculations.

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MÖSSBAUER STUDIES OF THREE ANTARCTIC METEORITES

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Antarctica is a unique location for meteorite discovery. The discovery of the first meteorite in Antarctica took place in 1912, but systematic searches began in the second half of the 20th century. To date, a total of 48,076 [1] registered meteorites have been found in Antarctica, with 1,845 originating from the Allan Hills region [1] (ALH meteorites). These meteorites, though found in the same region, do not come from a single fall and do not share a common parent body. ALH meteorites include various types such as aubrite, enstatite chondrites, lunar meteorites, and Martian meteorites, with ordinary chondrites being the most numerous group.

For ordinary chondrites, belonging to the category of stony meteorites, iron content ranges from 19 to 30 wt% of the total weight of the meteorite. Mössbauer spectroscopy proves to be a useful tool in meteorite research [2], especially when the specimens found are of small sizes. In this study, the results of Mössbauer spectroscopy conducted on three ordinary chondrites found in the Allan Hills region: ALH 88017 (type H4), ALH 88020 (type H3.5), and ALH 88021 (type H5) will be presented. Our research aims to gain a deeper understanding of the mineral composition and thermal history of these ordinary chondrites.

Keywords: meteorites, ordinary chondrites, Antarctic meteorites.

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AIR SCINTILLATION DETECTOR FOR CONVERSION ELECTRON MÖSSBAUER SPECTROSCOPY

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Conversion electron Mössbauer spectroscopy (CEMS) uses a variety of detectors based on different physical principles. Depending on the physical principle used, the detectors differ in design and application [1]. Proportional gas detectors using a He+CH₄ mixture as the working gas are most commonly used for room temperature measurements. The use of these detectors is limited by the need to place the sample in the detector space, which in turn limits the size of the samples that can be studied. The detector, based on the registration of light pulses produced by microbursts in air caused by electrons in the presence of an electric field, was described in [2]. This detector has been refined and used for CEMS measurements on a wide variety of samples. For example, steel samples annealed in different atmospheres and at different temperatures [3], sputtered alloy thin films on glass substrates, zinc ferrite nanoparticle coatings on austenitic alloy steel [4], CuFeO₂ thin films produced by high frequency reactive sputtering [5] and meteorites. It has been shown that the detector can be used to study both conducting and non-conducting samples. Comparison of CEMS and CXMS (Conversion X-ray Mössbauer Spectroscopy) confirmed that this is indeed a conversion electron registration, i.e. CEMS spectra carry information about a thin surface layer (about 300 nm). The advantage of the detector is that there are no restrictions on the size and partly on the form of the samples examined. At the same time, a certain shortcoming related to the tangential direction of incidence of gamma rays on the sample has been demonstrated. It has been shown that in some cases the resulting CEMS spectrum can be affected by the surface roughness of the sample. This was confirmed by comparing the CEMS spectra recorded by the air scintillation detector and the proportional gas detector.

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FROM LIGHT TO INSIGHT: EXPLORING BIOMOLECULAR STRUCTURES VIA RAMAN OPTICAL ACTIVITY

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Last year marked the 50th anniversary of a pivotal article in the journal *Nature*, which heralded the inception of vibrational chiroptical spectroscopy. This groundbreaking work documented the inaugural successful measurement of Raman optical activity (ROA) of molecular origin[1], validating the theory proposed by Professor Laurence Barron. Despite its inherent weakness and formidable measurement challenges, the ROA technique has experienced significant advancements over subsequent decades. A notable milestone occurred in the early 2000s with the introduction of the first commercially available ROA spectrometer, based on the pioneering design by Professor Werner Hug[2]. This transition propelled ROA from a tool primarily confined to fundamental research into a vital method for characterizing molecular configurations in industries like pharmaceuticals. Nevertheless, ongoing efforts continue to refine and broaden its application in fundamental research. Leveraging its remarkable capacity for extracting detailed structural information, particularly when integrated with precise quantum mechanical simulations incorporating electron correlation effects, ROA continues to yield invaluable insights into the structures of biologically active molecules and biomacromolecules.

In our contribution, we substantiate this assertion through a series of recent findings from our research group. These encompass (i) discerning manifestations of diverse sources of chirality, (ii) characterizing deuteration-induced chirality in pharmacologically active compounds, (iii) identifying sulfation-induced alterations in secondary structures of polysaccharides, (iv) delineating solvent-induced changes in secondary structures of polyproline helices, and (v) elucidating the characteristics of chiral supramolecular assemblies.

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RAMAN OPTICAL ACTIVITY AS AN IMPORTANT SPECTROSCOPIC TOOL IN THE STUDY OF THE STRUCTURE AND INTERACTIONS OF CHIRAL MOLECULES - CELEBRATING 50 YEARS OF DISCOVERY

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Raman optical activity is a chiroptical spectroscopic technique that was discovered 50 years ago[1]. Since then it has been established as a useful tool to provide information that is not readily available by other methods. This talk will review several areas that have been explored in our laboratory.

The optical purity of a chiral sample is of particular importance to the analytical chemistry and pharmaceutical industries. A methodology for the determination of enantiomeric excess using Raman optical activity (ROA) achieved an accuracy of better than 0.1 % for neat liquid and 0.2 % for aqueous solution[2].

ROA is also increasingly being used to describe the structure of many molecules of biological significance, from illicit substances[3] and nucleic acids to metal complexes[4]. Raman optical activity (ROA) combined with ab initio and molecular dynamics simulations with a realistic solvent description provides not only population weights for individual conformer groups, but also detailed insight into the structure of the molecules and their interaction with the solvent.

For Raman optical activity, it is also possible to exploit the wide spectral range of 50–4500 cm^{-1} , allowing the observation of anharmonic effects and distinct features of intermolecular interactions[5].

These results demonstrate the great potential of ROA spectroscopy for the quantitative analysis of chiral molecular systems.

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EXPLORING MONONUCLEOTIDE G-QUADRUPLEXES THROUGH VIBRATIONAL AND CHIROPTICAL SPECTROSCOPY

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The tendency of guanosine-5'-monophosphate (5'-GMP) to self-associate at higher concentrations has been known for over 100 years. The resulting agglomerates are called mononucleotide G-quadruplexes (mG4), which currently attract considerable research attention, especially in bionanotechnology [1], and have also been discovered to be significant in genomics. Despite extensive research, many fundamental aspects of the functional, dynamical, and structural properties of mG4 remain unclear. These include structural differences associated with different stabilizing cations, regularity, and stability of mG4 structures, as well as the interconnection of H-bonds in the outer part of mG4, along with helicity and ordering of G-quartets [2].

We employed Raman optical activity (ROA) and Raman scattering to monitor the self-association process of 5'-GMP. The well-resolved Raman and ROA spectra recorded across the whole range of fundamental vibrations bear significant information about mG4 structural properties. The observed spectral features, mainly sharpening and increasing intensity of vibrational bands, indicate that the ROA signal is highly sensitive and specific to different types of mG4 topology. Particularly, the THz region ($<200\text{ cm}^{-1}$), reflecting a higher-order arrangement, was found sensitive and distinctive to agglomeration with different stabilizing central cations. Furthermore, we discovered a significant reduction in the stability of mG4 (a drop in melting point of approximately 30°C) upon the replacement of ribose with 2'-deoxyribose, highlighting the crucial role of the H-bond network in mG4 stabilization. Our experimental data were supported by molecular dynamics simulations and advanced quantum mechanical calculations.

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ARE HYDRATION AND DYNAMICS FACTORS INFLUENCING THE ACTIVITY OF ENZYMES? INSIGHTS BY COMBINING TWO FLUORESCENCE TECHNIQUES WITH MD SIMULATIONS

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The hydration and mobility of proteins are believed to profoundly affect their function. However, only a few experimental approaches for monitoring these characteristics within the relevant protein regions are available. Here we describe two fluorescence methods for site-specific analysis of the extent of hydration and degree of the mobility in enzyme class of haloalkane dehalogenases. The first approach is based on recording time dependent fluorescence shift (TDFS) [1] placing the dye in the tunnel mouth of this enzyme [2]. Secondly, the „gating“ dynamics of the enzymes can be traced by fluorescence correlation spectroscopy following the photoinduced electron transfer (PET-FCS) between the selected tryptophan and properly positioned fluorescence dye [3]. The hydration and dynamics monitored within the biologically relevant regions of the dehalogenase enzymes is then compared with the enantioselectivity as well as catalytic efficiency of various mutants, which brings fundamental insights into the functioning of such enzymes. The fluorescence experiments are paralleled by MD simulations which are essential for setting up the experiments and interpreting their results.

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PLASMONIC METAL NANOPARTICLES WITH A RESPONSE IN THE NEAR-INFRARED REGION

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Nanomaterials are objects of intensive study due to their unique physical and chemical properties that open new possibilities for their application in various fields, like electronics, catalysis, sensorics, medicine, engineering, etc. This stimulates the development of new synthesis techniques, both physical and chemical, that allow for the design of nanomaterials with the required properties. Special attention is paid to the design of green methods that are based on the utilization of non-toxic compounds, often compounds of biological origin. This opens up an opportunity for its use in nanomedicine due to its biocompatibility.

A unique feature of metal nanoparticles is that their localized surface plasmon resonance wavelength position can be tuned by changing the size, shape, composition, and environment in accordance with the purpose of the utilization.

In this report, we present examples of changing the resonance absorption position by using nanoparticles with different shapes and dimensions. The UV-Vis-NIR properties of colloidal solutions of triangular and hexagonal gold nanostructures obtained with extracts of peppermint *Mentha piperita* L. [1] and goldenrod *Solidago canadensis* L. [2] were compared with the results of computer modeling of light absorption. The spectral position of localized plasmonic excitations of the studied nanostructures ranged from 520 nm for spherical gold nanoparticles to >800 nm for irregular gold nanoparticles. Photothermal studies of nanocolloid solutions have shown them as a prospective photothermal treatment agent [3].

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APPLICATION OF SENSOR ARRAYS FOR DETERMINATION OF EQUILIBRIUM CONSTANTS

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Chemosensor arrays are assemblies of multiple chemosensors where a single chemosensor should exhibit the highest selectivity to give the highest response (analytical signal) for a single analyte [1-3]. On the contrary, the methodology using arrays consisting of less selective chemosensor elements is more general because each element responds to more analytes present in the sample [1-3]. Thus, this overall analytical signal can be decomposed into individual signals originating from the analytes using advanced chemometrics methods. In this oral contribution, the digital-scanner technology for sensor arrays based on a microtiter plate(s) has been applied to get analytical signals followed by their evaluation to calculate the protonation constants of chosen compounds, *e.g.* methyl-orange, methyl-red, p-nitrophenol, 2,6-dichlorophenol. Their change in presence of different cyclodextrin-host molecules was utilized for estimation of binding constants of the supramolecular inclusion complexes. The obtained informations have been utilized for optimization of experimental conditions for the quantitative analysis of amantadine in drugs using this Indicator Displacement Analytical method.

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ENHANCEMENT OF LUMINESCENCE SIGNAL BY DEUTERATED WATER – ANALYTICAL APPLICATIONS

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The enhancement of luminescence signals through the substitution of water, which is the most common solvent, with deuterated water (D₂O) presents a transformative approach in chemical and biological research. This study investigates the impact of D₂O on fluorescence properties and its applications across diverse analytical methods, aiming to improve sensitivity and detection limits for a wide range of compounds. Experimental findings demonstrate that D₂O substitution amplifies fluorescence intensity and lifetime^[1], which can be beneficial for various samples such as dyes, labels, probes, biomolecules, and pharmaceuticals. Moreover, the utility of D₂O is showcased in optimizing analytical techniques including capillary electrophoresis with fluorescence detection (CE-LIF), high-performance liquid chromatography (HPLC)^[2], flow cytometry, fluorescence microscopy, fluorescence correlation spectroscopy, fluorescence-lifetime imaging microscopy (FLIM)^[3] and other. Incorporating D₂O into these methods leads to remarkable improvements in sensitivity and resolution, particularly evident in drug analysis and biomolecular studies. This research highlights the impact of deuterated water on advancing analytical methodologies, offering new possibilities for drug discovery, biomedical research, and environmental monitoring.

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EVALUATION OF CHARRING INFLUENCE ON THE CARBON, NITROGEN AND OXYGEN STABLE ISOTOPE RATIOS IN ARCHAEOBOTANICAL REMAINS

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Charred cereal grains are often found at archaeological sites. Stable isotopes of carbon, nitrogen and oxygen became a powerful tool in archaeological research; ratio of carbon stable isotopes (¹³C/¹²C) could provide information about environmental conditions [1] and about types of plants grown by ancient societies, nitrogen isotopes (¹⁵N/¹⁴N) could be used for the estimation of soil fertility and possible fertilization [2], and also for evaluation of dietary habits [3], and oxygen isotopes (¹⁸O/¹⁶O) allow reconstruction of past hydrological conditions [4].

The cereal grains found are generally charred, but the influence of the charring process on the isotopic ratios is not completely clarified. Therefore, our study focused on monitoring of changes in carbon, nitrogen, and oxygen isotopic ratios as well as of their content in grains subjected to accelerated charring. Three varieties of grains (einkorn, emmer and millet) were subjected to the influence of elevated temperature for a period ranging from 15 min to 48 hours under aerobic and anaerobic conditions. On the basis of thermogravimetric analysis, three temperatures (300, 450 and 550 °C) were selected.

The results obtained show that the isotopic ratios of elements under study at a temperature of 300 °C remain almost unchanged, on the other side at 550 °C the changes are quite remarkable.

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INTERACTION OF ZINC OXIDE NANOPARTICLES WITH SLOVAK SOILS AND THEIR SOIL COLLOIDS

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The behavior of nanoparticles (NPs) with natural soils and soil colloids, the most reactive part of soils, is of great interest. Interaction with the colloids with different properties, such as pH, content of natural organic matter, clay content and small sized oxyhydroxides of Fe may largely affect the behavior of zinc oxide NPs (ZnO-NPs) in soils and their colloids collected in temperate climate of central Europe, in Slovakia. Sequential centrifugation and centrifugal ultrafiltration were used on soil and soil colloids to find the distribution of Zn and other elements of interest in different size fractions. The concentration of zinc (Zn) in different size fractions was assessed in supernatant solutions obtained from centrifuged soil suspensions, providing a comprehensive understanding of ZnO-NP distribution and interaction across various soil characteristics. The study reveals that soil pH significantly affects the solid-liquid distribution of Zn in diverse forms, pointing to pH as the paramount factor in ZnO-NP distribution. Moreover, ZnO-NP changed distribution was also related to soil phosphorus (P) content. These findings have substantial implications for the environmental application and management of NPs, aiding in better prediction and simulation of NP behavior in soils of different properties. These insights into the behavior of ZnO-NPs in soils can contribute to the development of safer and more efficient NP-based applications in the field of environmental science and agriculture.

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LA-ICP-MS: AN INTERESTING TOOL FOR THE DETERMINATION OF SPECIFIC PROTEINS

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Determination of specific proteins is the key to the understanding of processes in the organism or development of diseases. Unfortunately, the determination of heteroatoms as P, S, Fe, Cu, Zn is insufficient for this purpose. Hence, the biorecognition tools for their determination by LA-ICP-MS are being developed. The most promising tool is based on the labelling of antibodies by nanoparticles. Their development and utilization for biological samples in combination with LA-ICP-MS analysis will be presented.

INVESTIGATIONS OF DOPED IRON OXIDE NANOPARTICLES BY MÖSSBAUER SPECTROSCOPY AND OTHER TECHNIQUES

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Iron oxides are important minerals (iron ores) and important synthetic materials used in various applications (pigments, catalysts, photocatalysts, adsorbents, magnetic materials, etc.). Natural iron oxides usually contain a certain amount of metal cations other than iron incorporated into their crystal structure, while the synthetic iron oxides are often intentionally doped with various metal cations in order to improve specific properties important for their applications. Doped iron oxides in the form of nanoparticles or nanostructured thin films can be prepared by different chemical or physical methods. Well-defined doped iron oxide nanoparticles are usually synthesized using hydrothermal or solvothermal precipitation methods.

In this lecture, the synthesis of pure and doped iron oxides goethite (α -FeOOH) and hematite (α -Fe₂O₃) nanoparticles by hydrothermal co-precipitation methods will be described. The results of investigations of the influence of doping with different metal cations on the structural, magnetic, thermal, vibrational, optical and photocatalytic properties of prepared iron oxide nanoparticles using ⁵⁷Fe Mössbauer spectroscopy and other techniques [1-3], will be presented and discussed.

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THE RELATIONSHIP BETWEEN STRUCTURE AND PHOTOCATALYTIC EFFECT OF LANTHANIDE-SUBSTITUTED GOETHITE NANOPARTICLES

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Goethite (α -FeOOH) is a stable iron oxyhydroxide and is abundant in nature. The goethites containing different elements substituted for iron have been extensively investigated for developing an effective photocatalyst^[1]. In this study, La-, Gd-, and Lu-substituted goethite nanoparticles (NPs) with substitution ratios from $x=0$ to 50 mol%, abbreviated as Lnx, were prepared by hydrothermal reaction. The local structure and the photocatalytic ability of the Lnx were investigated by ⁵⁷Fe-Mössbauer spectroscopy (FeMS), X-ray Diffractometry (XRD), X-ray Absorption Fine Structure (XAFS), Brunauer-Emmett-Teller (BET) method, and UV-Vis spectroscopy. The XRD patterns of Lnx showed a crystalline phase mainly derived from α -FeOOH in all samples, but an increase in the peak intensity due to La(OH)₃ and Gd(OH)₃, respectively, was observed from the XRD pattern of Lax and Gdx with x equal to or larger than 10 mol%, while that of Lux did not show Lu(OH)₃. The FeMS of α -FeOOH NPs is composed of two sextets with isomer shift (IS), quadrupole splitting (QS) and internal magnetic field (H_{int}) of $0.36_{\pm 0.01}$ mm s⁻¹, $-0.14_{\pm 0.01}$ mm s⁻¹ and $30.5_{\pm 0.5}$ T for the first, $0.36_{\pm 0.01}$ mm s⁻¹, $-0.21_{\pm 0.02}$ mm s⁻¹ and $35.9_{\pm 0.5}$ T for the second sextet, respectively. In addition, a doublet with IS of $0.35_{\pm 0.02}$ mm s⁻¹ and QS of $1.60_{\pm 0.03}$ mm s⁻¹ due to a superparamagnetic component was found. With the increase of the amount of La, Gd, and Lu, the absorption area (A) of the sextets decreased, while that of the doublet increased due to nanoparticulation. The specific surface area (SSA) of α -FeOOH was only 40.4 m² g⁻¹; increases in SSAs to 48.8 , 90.0 and 202.0 m² g⁻¹ were recorded for La 5, Gd20 and Lu20, respectively, due to the nanoparticles. In the methylene blue (MB) decomposition test, the reaction rate constant (k) decreased from $6.9 \times 10^{-3}_{\pm 0.3}$ to $2.6 \times 10^{-3}_{\pm 0.2}$ min⁻¹, to $3.1 \times 10^{-3}_{\pm 0.1}$ min⁻¹ and to $1.6 \times 10^{-3}_{\pm 0.1}$ min⁻¹ observed for Lax, Gdx and Lux with x from 0 to 50, respectively. It is concluded that decreases in the k values with the concentration of Lns are caused by the decrease in the goethite content and the formation of hydroxides.

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ANALYSES OF PRECIPITATES FROM THE TĚŠÍKOV ACIDULOUS WATER

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Analyses of precipitates and sediments obtained from Těšíkov acidulous water (Olomouc region, Czech Republic) were carried out by using of ⁵⁷Fe Mössbauer spectroscopy, X-ray powder diffraction, physisorption, atomic absorption spectroscopy (AAS) and scanning electron microscopy. While precipitates, which were obtained by direct drying of the water in Petri dish, contain dominantly crystalline calcium carbonate (CaCO₃), sediments taken from a close surroundings of the spring showed a presence of significant amount of iron containing phase. Particularly, the analyses of the sediments proved amorphous ferric oxide or oxyhydroxide nanoparticles with specific surface area of 190 m²/g. Mössbauer spectrum, which was measured at 5 K, was fitted only by one symmetrical sextet component confirming amorphicity and speromagnetic behavior of the analyzed sample [1]. In addition to iron containing phase and calcium carbonate, the sediment contained Si as well accordingly to Energy dispersive X-ray spectroscopy and AAS. Finally, the sediments obtained from the Těšíkov acidulous water present an easily accessible source of iron containing small nanoparticles, which can be further modified (e.g. by heating, coating etc.) with respect to their considered applications. In the presented study, a heating of the sediment samples at 400 °C in air resulted to formation of α-Fe₂O₃ nanoparticles.

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The image features a solid red background. At the top, there is a white, jagged, mountain-like shape that spans the width of the page. The shape has three distinct peaks of varying heights. In the bottom right corner, the words "POSTER" and "ABSTRACTS" are written in a white, bold, sans-serif font, stacked vertically.

POSTER
ABSTRACTS

EVALUATION OF KINETIC AND THERMODYNAMIC MODELS FOR METHYLENE BLUE ADSORPTION ONTO SAWDUST OF SPRUCE

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Numerous waste materials have been examined as potential candidates for the efficient and environmentally friendly removal of potentially hazardous substances. Considering that the temperature of the solution containing the adsorbate influences both kinetic and thermodynamic parameters, we have reexamined some of the most commonly used models to evaluate the suitability of spruce sawdust (*Picea abies*) as a potential adsorbent for removing methylene blue. Employing UV-VIS spectroscopy to collect concentration data (methylene blue exhibits its absorption maximum at 668 nm), we statistically analyzed the sorption kinetics across various temperatures (ranging from 298 K to 338 K) and initial concentrations (from 10 mg·L⁻¹ to 300 mg·L⁻¹). The data revealed a linear increase in rate constants over the temperature range considered (for example, from 0.033 min⁻¹ at 298 K to 0.151 min⁻¹ at 338 K for the pseudo-first order kinetic constant). However, the effect of adsorbate concentration on rate constant exhibited two distinct phases. In the first phase, below an initial methylene blue concentration of 50 mg·L⁻¹, there was a rapid decrease in the kinetic constant value. In the second phase, the value increased, with the temperature having a variable effect on the magnitude of the increase. These findings underscore the mutual influence of initial concentration and temperature on the kinetics of methylene blue adsorption onto spruce sawdust, offering new insights into the mechanisms that enable the removal of this environmentally hazardous material from contaminated industrial effluents.

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APPLICATION OF AN ATMOSPHERIC PRESSURE GLOW DISCHARGE-LIKE (APGD) BASED HYDRIDE ATOMIZER TO DETERMINATION OF As AND Se BY AAS

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Atmospheric pressure glow discharges (APGDs) are non-equilibrium gas discharges formed between two electrodes powered by high voltage (~ 1-10 kV). The discharge current is typically in the range of 10-100 mA, and the discharge gap varies from 1 to 5 mm. The high gas temperature and electron number density, which are 1500-3500 K and 10^{14} - 10^{15} cm⁻³, respectively, predetermine the APGDs to be used as promising atomizers to be used in trace element analysis performed by atomic spectrometry. The most common approach is to couple APGD with optical emission spectrometry. Much less explored is the use of APGD as a source of free atoms for atomic absorption spectrometry (AAS). Several analytically important elements including As, Se, Sb, Bi, Te, Sn, Pb, Bi and Ge can be converted to corresponding hydrides prior to their detection by AAS resulting in enhanced analyte introduction efficiency and reduced risk of interferences when compared to sample introduction by liquid nebulization. The most common hydride atomizers in AAS include externally heated quartz tubes (QTA). In last decade, plasma atomizers based on dielectric barrier discharge (DBD) have been successfully used for determination of As, Se, Sb and Te, while reaching not satisfactory sensitivity for Bi, Pb, Sn and Ge. The motivation of this work was to explore the potential of APGD hydride atomizers for AAS.

An APGD atomizer was constructed making use of the quartz body of a QTA atomizer. However, instead of resistive heating of the optical arm, two electrodes were inserted in its central part to sustain an APGD-like discharge (0.5 kV, 30 mA). Atomization of As and Se hydrides was optimized. The effect of discharge gas nature (Ar, He) and flow rate as well as the power supply rate on analyte signal has been investigated. Subsequently, analytical figures of merit such as sensitivity and limits of detection (LOD) were determined under optimum operation conditions. The sensitivity values ranged between 0.3 and 0.4 s ng⁻¹ while the LODs were quantified to 0.14 ng ml⁻¹ As and 0.11 ng ml⁻¹ Se. The performance of APGD hydride atomizer is comparable in case of As and Se to that of QTA or DBD atomizers. Applicability of APGD atomizer to other hydride forming elements such as Sb, Pb or Sn will be outlined.

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A NOVEL VORTEX–ASSISTED LIQUID–LIQUID MICROEXTRACTION BASED ON DEEP EUTECTIC SOLVENT FOR THE SEPARATION, PRECONCENTRATION AND DETERMINATION OF RHODAMINE B IN WATER SAMPLES

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A new green, highly sensitive and simple method based on vortex liquid-liquid microextraction (VALLME) using deep eutectic solvents (DES) was developed for the UV-Vis and spectrofluorimetric determination of Rhodamine B (RhB). DES are a promising alternative to common conventional organic solvents and play an important role in analytical chemistry by improving sample handling and being environmentally friendly. The aim of this work was to show the advantages of DES on the example of the determination of the organic dye RhB, which is commonly used as a fluorochrome.

UV-Vis measurements were carried out at a maximum wavelength of 555 nm. Fluorescence intensity was measured in the wavelength range of 500-700 nm at an excitation wavelength of 555 nm with a peak around 574 nm. The experimental conditions of extraction were optimized and found to be 100 μL of DES as extraction solvent, vortexing, 15 s at 2000 rpm, and centrifugation, 3 min at 1500 rpm. In our study, we compared the analytical properties of conventional solvents (n-amyl acetate, octanol, toluene, chloroform and tetrachloromethane) and DES prepared by mixing tetrabutylammonium bromide (TBA)Br with alcohols (hexanol, octanol, decanol) in different ratios (1:1, 1: 2, 1:3). The efficiencies of individual DES were higher or comparable to other organic solvents, while the highest value of the fluorescence intensity of the extracts was achieved by the DES composed of (TBA)Br and hexanol in a ratio of 1:3.

The linearity of the calibration dependence was observed in the RhB concentration range from 0 to 10 $\mu\text{g L}^{-1}$ ($R^2 = 0.9991$). The limit of detection (LOD) was 0.023 $\mu\text{g L}^{-1}$. Preconcentration factor (PF) and enrichment factor (EF) were determined to characterize the efficiency of the microextraction method, which corresponded to the values of 50 and 58. The accuracy and correctness of the proposed method was verified during two consecutive days with RSD values of 3.2-4.1% and recovery of 92.6-103.5%. To demonstrate the practicality of the proposed procedure, a method was applied to the determination of RhB in a real water samples was developed.

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A GREEN ULTRASENSITIVE FLUORESCENCE DETERMINATION OF ANIONIC SURFACTANTS WITH THE USE OF VORTEX-ASSISTED LIQUID-LIQUID MICROEXTRACTION

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Anionic surfactants are effective and inexpensive, which is why they are used in personal care products such as soaps, toothpastes, shampoos, and shower gels, but also in household cleaning products, especially laundry detergents and floor cleaners. Because a variety of anionic surfactants occurs in environmental samples, it is necessary to determine the total concentration of such compounds using a recalculation through a base substance, as a rule, sodium dodecyl sulfate (SDS).

We developed a new method which is based on the reaction of SDS with the 3,3'-diethyloxadicyanone iodide (DODC) dye, followed by vortex-assisted liquid-liquid microextraction (VALLME) of the resulting ion associate (IA) into a microvolume of n-amyl acetate (70 μ l). The DODC dye was used for the first time in the analysis as an effective fluorophore and at the same time an effective extraction reagent. The fluorescence intensity of n-amyl acetate extracts of IA increases with increasing concentration of anionic surfactants. The calibration curve was linear over the anionic surfactant concentration range, 0.30 to 3.0 μ g L⁻¹, $R^2 = 0.9980$. Vortex-assisted microextraction ensures a high concentration and enrichment factor, which, in combination with a sensitive fluorescence detection technique, is the basis for achieving an LOD of 0.10 μ g L⁻¹ of anionic surfactants.

Our effort was to develop a simple and sensitive method that would meet the requirements of green analytical chemistry. The amounts of used chemicals and organic solvents were minimized down to micro-volumes, thanks to which the method meets the requirements of green chemistry. Evaluation of the proposed method from the perspective of green analytical chemistry was carried out using green evaluation metrics such as Analytical Greenness Comprehensive Tools (AGREE) and Green Analytical Procedure Index (GAPI). Our proposed method achieved a score of 0.84 according to the AGREE method.

To demonstrate the practicality of the proposed procedure, a method for the determination of anionic surfactants in real water samples (water, river and waste water) was developed and applied. Satisfactory recovery data ranging from 93.3 to 106.7% were obtained, with a relative standard deviation of 2.2 to 4.9%.

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UV-PHOTOCHEMICAL VAPOUR GENERATION OF SILVER: STUDY OF CONDITIONS

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The first UV photochemical generation of silver was performed by Guo et.al.¹ Their conclusion was that silver appears to be amendable to UV-photochemical vapour generation method as a sample introduction system, however the very noisy signals achieved suggested that the compounds created were unstable. Our work addresses the search for optimum conditions for generation of volatile species of silver and its mechanism. We found that the reduction of silver is relatively simple, but it's reduced to metal form rather than volatile species. The most direct and rapid transport in the system is required for successful generation of a volatile species, so the emphasis has been on the experimental setup, shortening of the and reducing the number of connection points. Flow injection mode was used in conjunction with ICP-MS detection and silver was detected on mass 107 in time resolved analysis. Obtained signals were mainly dependent on the type of low molecular weight acid used, on its concentration, on sample and carrier gas flow rate and on positioning of carrier gas inlet. Attention was also paid to the construction of gas-liquid separator.

We confirmed that the response belongs to volatile species not to aerosol, and that the volatile species arise due to action of UV radiation and not due to heat transmission. For better understanding of mechanism of UV-PVG generation, signals obtained with solution of ionic standard were compared to signals acquired with solution containing silver nanoparticles.

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ATOMIZATION OF HYDRIDE-FORMING ELEMENTS IN ATMOSPHERIC-PRESSURE DISCHARGES

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The coupling of a hydride generation to atomic absorption or fluorescence spectrometry is a well-known method to trace element and speciation analysis. It enables efficient and “matrix-free” analyte introduction into the detector. Heated quartz tube atomizers or diffusion flames are the most common hydride atomizers. Nowadays also plasma atomizers based either on a dielectric barrier discharge or an atmospheric-pressure glow discharge (APGD) are reported as alternative hydride atomizers. The dielectric barrier discharge is capable of efficient atomization of As, Se, Sb, and Bi hydrides while reaching poor sensitivity for Pb, Sn, and Ge. Apart from dielectric barrier discharge, Ge is detected with low sensitivity even in the most common hydride atomizers.

As a consequence, an APGD-based atomizer was investigated in this work to overcome the low sensitivity observed in dielectric barrier discharge for elements as mentioned above. Several APGD designs were developed and tested using As, Se, and Ge. The first APGD construction resembled the design of the diffusion flame. However, the discharge was unstable and suffered from low sensitivity due to a short optical path. The other two APGD designs tested were derived from the quartz tube atomizer. In the first arrangement, analyte hydride was introduced through a quartz capillary in a parallel direction with the plasma. In the second arrangement, analyte hydride was introduced through a inlet arm perpendicularly to the plasma and the electrodes. The latter was selected as the best design its performance was compared to other hydride atomizers. The current-voltage characteristics of the APGD power supply sources were also measured.

Moreover, the distribution and absolute concentration of hydrogen radicals/free analyte atoms in the APGD were studied by two-photon/laser-induced fluorescence, and the results will be correlated with atomic absorption spectrometry experiments.

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COUPLING OF MINIATURIZED UV-PHOTOCHEMICAL VAPOR GENERATION REACTOR WITH SEQUENTIAL INJECTION ANALYSIS

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UV-photochemical generation of volatile species (UV-PVG) is a novel and promising technique increasing sample introduction efficiency in atomic spectrometry and can be used for a broad range of elements.¹ Currently, the flow injection systems in use are mostly based on bulky photoreactors. One of critical parameters is irradiation time, which in flow reactors can be controlled only by the flow rate. Using miniaturized photoreactor based on pen-ray lamp and coupling it with sequential injection analysis (SIA) allows for precise control of irradiation (reaction time) by stopping the reaction zone in photoreactor. Additionally, by miniaturizing UV-photoreactor and coupling it with SIA, the consumption of chemicals can be reduced to a bare minimum.

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PLASMA SPECTROSCOPY IN LASER ABLATION SYNTHESIS OF NANOPARTICLES

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Pulsed laser ablation in liquid (PLAL) is one of the several methods used to synthesize nanoparticles (NPs). The main principle is laser ablation of a metal target immersed in liquid. The laser-matter interaction includes material vaporization, atomization, excitation, ionization, and laser-induced plasma (LIP) generation. In the case of a liquid environment, interaction is moreover connected with cavitation bubble formation associated with rapid plasma collapse.

The naked eye can usually observe the optical emission of generated plasma. Its spectroscopic study brings essential information about the laser ablation process. From this point of view, it is a specific variant of laser-induced breakdown spectroscopy (LIBS) with the sample surface under liquid; however, this use has only been explored a little.

This work deals with comparing the spectral characterization of LIP that was provided on different kinds of metal targets immersed in several solvents (water and organic solvents) and in the air. These comparisons are necessary to study due to various physical properties. Generated nanoparticles were separated, and their size distribution and chemical composition were determined.

The main issue of this work is to find the connection between the spectroscopic data and the properties of the generated NPs, which will also be presented in this work.

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ASSESSMENT OF MEPS FOR INORGANIC ANIONS DETERMINATION

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MEPS is a miniaturized version of solid-phase extraction introduced in 2004 [1]. This approach has found wide application in sample preparation with chromatographic finishing. The sorbent in MEPS is packed in a special cartridge in the form of a steel barrel placed in a needle and is called BIN. To the best of our knowledge, MEPS has not yet been used for the analysis of inorganic anions. We have assessed the possibility of using this technique for the determination of inorganic anions on the example of orthophosphate with subsequent spectrophotometric detection. The method is based on the formation of phosphomolibdenum blue (PMB), the formation of ion associate (IA) with cetyltrimethylammonium bromide (CTAB) and its sorption on BIN with C18. The IA was further eluted with acetonitrile and its absorbance was measured in a 10 mm microvolume cuvette. The procedure was carried out in semi-automated mode using digital syringe.

It was found that acetonitrile and acetone have good efficiency in eluting PMB. Methanol and ethanol give lower absorbance values. In acidified ethanol medium, there was a decrease in absorbance over time, which may be due to the degradation of PMB. It was found that the optimum eluent volume was 60 μ l and the elution process was better to be carried out three times with equal portions of 20 μ l. The optimal volume of HPB solution that needed to be passed through the sorbent to achieve the highest sensitivity was 4.5 mL (or 9 sorption cycles of 500 μ L PMB). Based on the obtained data, a sensitive method for the determination of phosphate in water was developed. For the analysis up to 5 ml of sample and 60 μ l of organic eluent is enough, that is much lower than in the standard method for phosphate determination (ISO 6878): sample volume up to 300 ml, hexanol volume - about 60 ml. LOD of the method was 0.4 μ g/l and RSD was in the range 4.5 – 13%.

Thus, the possibility of MEPS application for the analysis of inorganic anions with spectrophotometric detection is shown on the example of phosphate determination in water samples.

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INVESTIGATION OF SELENITE SORPTION ONTO MAGNETITE NANOPOWDER USING FLAME ATOMIC ABSORPTION SPECTROMETRY

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Selenium, which belongs to the basic elements, has a narrow border between necessity and toxicity [1]. Anthropogenic activities can lead to its increased concentrations in aquatic ecosystems, especially in the undesirable form of toxic selenite, due to its high environmental mobility [2]. In particular, magnetite-based nanomaterials have shown promise as sorbents due to their ability to immobilize contaminants through reductive transformation or adsorption [3]. The aim of this work was to study the sorption properties of magnetite nanopowder, to investigate critical factors such as pH, ionic strength and competing anions that affect selenite removal. Sorption kinetics revealed an initial rapid removal of selenite, followed by a slower, time-dependent phase. Chemisorption was considered to be the primary sorption interaction, with diffusion playing a minor role and best described by a pseudo-second-order kinetic model. In particular, pH significantly affected the sorption efficiency, with acidic conditions favoring selenite removal, while alkaline conditions decreased efficiency due to repulsive interactions. The equilibrium sorption data were best fit by a Langmuir model with maximum sorption at pH 3, indicating that acidic conditions favor selenite removal. Based on the obtained results, we assume that magnetite nanopowder is a sorbent suitable for removing selenium from wastewater in a wide pH range.

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STUDY OF MICROBIAL INDUCED STRUCTURAL TRANSFORMATION OF MAGNETITE BY MÖSSBAUER SPECTROMETRY

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Fungal biomass is used in various remedial technologies to enhance sorptive capabilities. However, it has limitations such as low affinity for negatively charged substances and slow sorption kinetics, necessitating modifications. In an aqueous environment, magnetite nanoparticles tend to agglomerate, hindering their sorptive properties. However, this issue can be effectively addressed through a suitable stabilization method. Synergistically combining magnetite with other materials makes it possible to modify and overcome their inherent disadvantageous properties. We investigated a new method in this study: cultivating *Aspergillus* spp. with magnetite nanopowder, resulting in the formation of pellet-like biomass structures containing the nanoparticles. The ideal method for detecting subtle changes from microscopic fungi in magnetite nanopowder is Mössbauer spectrometry [1], known for its sensitivity to iron nuclei, allowing precise identification of iron chemical species in the composite sorbent. Despite minimal structural alterations detected, *Aspergillus* spp. exhibited distinct behaviour in the presence of magnetite, retaining their mineralogical integrity.

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ENHANCEMENT OF ANALYTICAL POTENTIAL OF ETAAS: COMPARATIVE STUDY OF THREE EXTRACTION PROCEDURES USED FOR ULTRATRACE LEAD

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The aim of this study is to enhance the analytical potential of electrothermal atomic absorption spectrometry (ETAAS) for the quantification of ultratrace Pb. This goal was accomplished through the optimization of three extraction procedures: cloud point extraction (CPE), coacervative extraction (CAE), and dispersive solid-phase extraction (dSPE).

In CPE, the method relies on the extraction of the Pb-pyrrolidine dithiocarbamate complex into the surfactant-rich phase (SRP) containing the non-ionic surfactant Triton X-114. Following the separation of the aqueous bulk solution from the SRP, the final extract was diluted with 200 µL of acidified methanol. Under optimized conditions (using an initial sample volume of 10 mL), an EF of 28, a LOD of 0.08 µg/L, a LOQ of 0.28 µg/L, a RSD of 5.6% (for 2 µg/L of Pb; n = 18), and a linear calibration graph ranging from 0.3 to 2.8 µg/L were achieved.

In CAE, the method involves the extraction of the Pb-dithizone chelate with coacervates comprised of lauric acid in the presence of potassium ions and methanol. After separating the aqueous bulk solution from the SRP, the final extract was redissolved using 500 µL of acidified methanol. Under optimized conditions (using an initial sample volume of 10 mL), an EF of 17, a LOD of 0.12 µg/L, a LOQ of 0.40 µg/L, a RSD of 4.2% (for 2 µg/L of Pb; n = 26), and a linear calibration graph ranging from 0.4 to 4.5 µg/L were achieved.

In dSPE, the method is based on the adsorption of Pb onto nano-TiO₂, followed by direct TiO₂-slurry sampling into a graphite furnace. Under optimized conditions (using an initial sample volume of 50 mL, 50 mg of nano-TiO₂, and a final slurry volume of 5 mL), an EF of 10, a LOD of 0.14 µg/L, a LOQ of 0.48 µg/L, a RSD of 3.8% (for 4 µg/L of Pb; n = 30), and a linear calibration graph ranging from 0.5 to 8.0 µg/L were achieved.

All methods were validated by analyzing certified reference material (TMDA-61). Extraction recoveries for the CRM, spiked model solutions, and spiked natural water samples ranged from 88% to 106%. Ultimately, all methods were successfully applied to the separation/preconcentration and reliable quantification of ultratrace Pb in various natural water samples.

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LEGISLATIVE AND SAFETY LIMITS OF TOXIC ELEMENTS IN FOOD

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Many elements such as arsenic, chrome, tin, selenium, and other similar elements are well known as toxic elements or biogenic, depending on their concentration and which can occur in food in several different forms. These forms have different toxicity or other biological activity for humans, and therefore the determination of the total amount of these elements in food gives insufficient information [1].

As part of this work, a procedure for determining and specifying the elementary compounds in food samples such as drinks, fish, cereals, and other vegetable foods was created. The procedure included the use of high-performance liquid and ion chromatography methods (HPLC, IC) with atomic fluorescent spectrometry detection with hydride formation technique (HG-AFS) [2]. The comparison method was used by the Mass spectrometry method with inductive bound plasma (ICP-MS) to determine the overall elementary content.

Furthermore, this study deals with the analysis of 43 mineral elements on higher levels and trace levels in non-traditional wheat grains, flakes and undigested flake parts by means of ICP-MS and after the production of flakes decreases in the appropriate content [3]. It also identifies appropriate diet intake, in vitro digestibility, retention factors and metal pollution indexes [4].

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IODINE DETERMINATION IN CARROT BY ICP-MS

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Iodine is a vital micronutrient for most organisms, including humans. Despite extensive efforts through iodine deficiency disorder elimination programs, such as salt iodization, iodine deficiencies persist [1]. Subclinical deficiencies of iodine often exhibit an endemic nature and are characteristic of specific areas where iodine is deficient or inaccessible in the geochemical environment due to various factors, particularly in soil, drinking water, or food [2, 3]. Biofortification of crops with iodine, when applied in the correct chemical form, offers an attractive and cost-effective alternative approach to increasing daily iodine intake and combating iodine deficiency disorders [4].

Extraction and fractionation of naturally occurring iodine from environmental samples, followed by spectroscopic determination, is the most used method for iodine determination. Currently, iodine determination via inductively coupled mass spectrometry (ICP-MS) is the most prevalent and reliable method for determining total iodine content in environmental samples and foodstuffs [5].

In this study, iodine concentration and distribution were determined in various parts (leaves, stem, peel, and root) of carrots fortified with 100 mg.kg⁻¹ of iodide and iodate in soil. Iodine extraction using 25% tetramethylammonium hydroxide was followed by iodine determination using ICP-MS. The results indicate that iodate treatment is more effective for iodine fortification in carrot plants.

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UNCOVERING MAGNET COMPOSITION IN MODERN ELECTRONICS BY ICP-OES

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Lanthanoids, i.e. elements between La-Lu, are used in many areas. One of the most commonly encountered forms are magnets. Neodymium-based magnets, generally referred to as NdFeB, are the strongest commercially available magnets nowadays. As the name suggests, the composition is based on Nd, Fe and B, however, other lanthanoids are added to improve the properties, such as resistance to demagnetization at elevated temperatures. These include Pr, Tb, Dy, and less frequently other lanthanoids. Finally, Ni, Cu, V, Ti and Co can be present, in the magnetic material or its surface coating. [1, 2, 3]

Currently, the majority of the world's production of lanthanoids is situated in China. For ecological, economical, but also political reasons, there is an effort to introduce recycling of lanthanoids from used magnets. For example, Apple has promised that by 2025, 100 % of magnets in their devices will be made from recycled lanthanoids. [4] However, for development of recycling procedures, more information is needed about the magnet composition, which varies for different applications. Therefore, this work aims to present an insight into the elemental composition of magnets in various "everyday" items such as hard drive, tablet, headphones and others. The magnets were dissolved in HNO₃ or aqua regia and after dilution analyzed using a Spectro Arcos MV (Spectro Analytical Instruments, Germany) ICP-OES instrument in radial view. Spectral interferences were thoroughly checked and interfered emission lines were omitted from evaluation.

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THE USE OF THE RAMAN SPECTROSCOPY AND XRF SPECTROMETRY IN THE ENVIRONMENT OF THE NATURAL HISTORY MUSEUM.

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The contribution discusses the broad-spectrum use of Raman spectrometer (Thermo Scientific DXR3xi Raman Imaging microscope) and XRF spectrometer (ARL™ QUANT'X EDXRF Spectrometer) in the environment of Natural History Museum. In general, we can divide this topic into two main parts, the first is the use of instrumentation in the identification of Slovak National Museum – Natural History Museum collection objects of various types, such as: rocks used by man in the past (archaeology), artifacts related to human development (anthropology), jewelry (history) and in last but not least, minerals from our depositories (mineralogy). The second part is the use in scientific projects from applied research (impact of mining on the environment) to basic research (identification of new minerals).

Raman spectroscopy is incomparably the most suitable non-destructive method for identifying minerals in collection objects. We have successfully characterized minerals in historical jewelry, mineral coatings of anthropological items and variety of archeological objects. More challenging, but still effective is the identification of natural materials such as tortoiseshell and ivory.

XRF spectrometry appears as suitable tool for chemical analysis of variety of museum objects such as archeological items, historical pavings, plasters and many others. This method also allows us to do a cheap and detailed monitoring of the areas contaminated by ore mining and to construct detailed geochemical maps of potentially toxic elements distribution in soils and stream sediments.

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RAMAN AND EXAFS SPECTROSCOPY OF SYNTHETIC AND NATURAL COPPER OXALATE

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In a natural environment, copper oxalate hydrate is known as mineral moolooite. According to the most recent study [1], a formula for moolooite should be formulated as $\text{CuC}_2\text{O}_4 \cdot n\text{H}_2\text{O}$ since there is a variable amount of water incorporated into the crystal structure that maintains structural integrity. However, the amount of water that can be incorporated into the crystal structure seems to differ from sample to sample. Therefore, in this contribution, we present the Raman spectra of synthetic copper oxalate with excitation 532 nm ($<3400 \text{ cm}^{-1}$) and 785 nm ($<1800 \text{ cm}^{-1}$). In comparison, we also present the Raman spectra of natural copper oxalate of biogenic source (products of lichenized fungi) again, with excitation 532 nm ($<3400 \text{ cm}^{-1}$) and 785 nm ($<3400 \text{ cm}^{-1}$). On the same sample dataset, the extended X-ray absorption fine structure (EXAFS) spectroscopy was employed. This way, the reference spectra were obtained, which will secure the precise identification of this compound in difficult samples of microscopic sizes in a natural environment. The diagnostic Raman bands of synthetic copper oxalate are: 206s, 297, 555s, 582, 607, 827, 919, 1483, 1512vs, 1610, and 1660 cm^{-1} (with 532 nm excitation) and 209s, 298, 558s, 585, 610, 833, 922, 1483, 1514vs, 1612, and 1665 cm^{-1} (with 785 nm excitation). In comparison, diagnostic bands of natural copper oxalate are: 206, 288, 555, 582, 607, 827, 917, 1485, 1512, 1610, 1659, and a broad signal at 2926 cm^{-1} (with 532 nm excitation); and 210, 301, 558, 586, 613, 832, 923, 1485, 1515, 1615, 1669, and a broad signal at 2909 cm^{-1} (with 785 nm excitation). Broad bands at ca 2900 region in the spectra of natural oxalates suggest that natural copper oxalates are more hydrated than synthetic analogues. Application of EXAFS spectroscopy on samples well-characterised by Raman spectroscopy will improve the identification of copper oxalate from biogenic sources.

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SPECTROSCOPIC APPROACHES FOR ANALYSES OF IRRADIATED CONCRETE IN HOT CELLS

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The poster focuses on the hot cell infrastructure and its laboratory equipment used to pre-characterize irradiated bio-shielding related to concrete structures. The structures of nuclear power plants are subject to degradation due to the effects of neutron and gamma radiation as well as high temperatures [1]. Spectroscopic techniques such as SEM-EDX and X-ray diffraction help to study these degradation processes, such as microstructural change, change in chemical composition, volume expansion and crack propagation.

The handling of irradiated samples, which are radioactive, differs from non-irradiated samples, hence the emphasis on the actual pre-characterization, where possible difficulties in sample preparation and testing are eliminated. For these reasons, special infrastructures are used to study irradiated samples. Research Centre Rez Hot cells facility is a complex of hermetically sealed boxes in which samples are handled by fully mechanized manipulators. In addition to the hot cells, an associated semi-hot cell contains instruments more sensitive to high radiation.

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HIGH RESOLUTION SINGLE CELL LA-ICP-MS 2D IMAGING

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The gradual development of instrumentation and the incorporation of additional equipment has led to the expansion of the laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) into medical applications. Currently, this technique is making inroads into oncological research in the context of 2D soft tissue imaging. Nevertheless, conventional biomedical studies rely on large laser beam sampling (75–20 μm), which does not allow to provide high-resolution isotope distribution. However, the integration of innovative devices, such as rapid sample transport devices from the ablation cell or even rapid response cell designs for laser ablation, allows tracking ultra-trace amounts of analyte in femtogram samples.

This work focuses on the use of LA-ICP-MS for 2D-imaging of A549 cell line, a lung cancer epithelial cell line, injected with a newly synthesized unique potential agent based on ruthenium. A fundamental study of the laser ablation working parameters was performed, providing a detailed imaging of the distribution of the $^{101}\text{Ru}^+$ isotope with a resolution of 2 μm . In addition, trends in influx and efflux and agent distribution were monitored as a function of cell harvest time at 6, 12 and 24 hours after drug application. It was discovered that most of the agent was found in the cell samples taken at 12 hours after treatment and it was predicted that there is probably preferential accumulation of the drug in the nuclei of the cells.

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

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Polydopamine (PDA) serves as a widely employed anchoring layer across various applications; however, its utility can be restricted due to its notable chemical and topological variability. Understanding the formation process and physicochemical characteristics of the formed confluent layers and the adherent nanoaggregates [1] on a nanoscale level is essential for expanding the potential applications of PDA. Through the application of nano-FTIR spectroscopy, we examined PDA layers on three distinct substrates (silicon/silicon dioxide, nitrogen-doped titanium oxide, and gold) at various times of deposition (ToD). We identified a strong correlation between nano-FTIR and macroscopic FTIR spectra [2], reflecting alterations in the relative abundance of PDA and polymerization intermediates with increasing ToD. Furthermore, employing principal component analysis allowed for additional insights from loadings spectral curves and data distribution in score plots. Notably, we observed greater spectral variability in the ultrathin surface confluent layers compared to the adherent nanoaggregates. While nanoaggregate spectra displayed no discernible dependence on ToD or substrate material, the layer spectra were significantly influenced by both of these parameters, especially at the initial phases of the deposition process.

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MOSSBAUER AND MAGNETIC STUDIES ON NANOCRYSTALLINE FENI PARTICLES PREPARED BY THERMAL REDUCTION

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The development of technology in recent years requires cheap high-performance magnets. One of the promising candidates of rare-earth-free hard magnetic materials seems to be Fe-Ni-based alloys, especially L10-FeNi phases.

In this study, a promising method of thermal decomposition of oxalate precursor was investigated. Oxalate precursor particles were synthesized by the coprecipitates method and subsequently subjected to controlled thermal decomposition in a reducing hydrogen atmosphere for acquiring FeNi alloy particles. The physical characterization of the samples was carried out using Mössbauer spectrometry, X-ray diffraction, magnetization measurements, scanning electron microscopy, and energy dispersive X-ray spectroscopy.

X-ray diffraction and Mossbauer spectroscopy demonstrated the presence of a mixture of bcc phase alpha-Fe(Ni) and fcc iron-nickel phase in the sample after thermal decomposition. The results of Mossbauer showed the change in hyperfine parameters along with changing temperature.

Particles were approximately cube-shaped unit cell morphology with a size in the range of 1-2 μ m and contained several phases with variable Fe-Ni content. The magnetic measurements confirmed the formation of magnetically suitable Fe-Ni phases in the samples after annealing.

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SEASONAL AND SPATIAL VARIATIONS OF ARSENIC AND ITS SPECIES IN PARTICULATE MATTER IN BRNO CITY

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The present study deals with an analysis of total arsenic concentration using ICP-MS/MS and an analysis of concentration of several arsenic species – arsenite (As^{III}), arsenate (As^{V}), monomethylarsonate (MMA), dimethylarsenite (DMA) and trimethylarsineoxide (TMAO), using HPLC-ICP-MS/MS in the PM_{10} fraction of airborne urban aerosol. The samples were collected at three locations within the central European city of Brno, with the aim to evaluate a spatial influence of potential sources of PM. To gain better understanding of the arsenic origin, an analysis of the total arsenic concentrations was performed in samples of different size fractions of particulate matter collected using ELPI+. To evaluate seasonal variations, the sampling was repeated in two campaigns, specifically in the autumn of 2022 and in the winter of 2023. The results confirmed both spatial and seasonal variability in the content of the methylated arsenic species in PM_{10} influenced by biomethylation processes. The predominant source contributing to the total As content in PM_{10} was identified as local emissions, including industrial activities and heating during the winter season.


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MANGANESE BIOEXTRACTION POTENTIAL OF MICROSCOPIC FILAMENTOUS FUNGUS

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Manganese is a transition metal that is the 10th most abundant chemical element on Earth and makes up to 0.1% of the Earth's crust. It is a structural component of more than 250 minerals and, in the case of several other minerals, is a substituent of Fe²⁺ and Mg²⁺ cations [1].

Manganese occurs in various oxidation states of which the +II, +III and +IV are predominant under natural conditions [2].

Manganese oxides and (oxo)hydroxides are among the most common secondary minerals of manganese in the soil. These are reactive phases that play an important role in the geochemical cycling of various elements [3].

This study aimed to examine the bioextraction of manganese oxides at various oxidation states (MnO, Mn₃O₄, Mn₂O₃ and MnO₂) by a strain of the filamentous fungus *Aspergillus niger*, a frequent soil representative. Our results showed that the fungus effectively disintegrated the crystal structure of selected mineral manganese phases. Thereby, during a 31-day static incubation of oxides in the presence of fungus, manganese was bioextracted into the culture medium and, in some cases, transformed into a new biogenic mineral. The Mn(II,III)-oxide was the most susceptible to fungal biodeterioration, and up to 26% of the manganese content in oxide was extracted by the fungus into the medium. The culture media filtrates were analyzed for the total manganese content by flame atomic absorption spectroscopy (F AAS) at line Mn 279.5 nm using an AAS spectrometer Perkin-Elmer Model 1100 (Perkin-Elmer, Uberlingen, Germany). Deuterium background correction was used.

Our results highlight the significance of fungal activity in manganese mobilization and transformation. The soil fungi should be considered an important geoactive agent that affects the stability of natural geochemical barriers.

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MULTIFERROIC BaYFeO₄: FABRICATION AND INVESTIGATION BY MÖSSBAUER SPECTROSCOPY

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BaYFeO₄ ferrite was reported to possess spin-driven ferroelectricity and magnetoelectric coupling [1]. Such a type of material might have significant potential for the application of future electronic devices.

High-quality BaYFeO₄ samples are synthesized using a conventional solid-state reaction method in air. First, we transfer BaCO₃, Y₂O₃ and Fe(NO₃)₃ into nitrate solution. The precipitate of the oxalates was formed after adding oxalic acid, which was then dried and heated up to 700 °C for 12 h in air. The mixture was ground and heated at 1050 °C for 16 h. The sample was ground, pressed into pellets, and heated several times at temperature from the range 1250 – 1325 °C until a pure phase sample was obtained.

An alternative approach to the preparation of BaYFeO₄ is a ball milling of the initial oxides. The samples were prepared depending on the different milling time, $t = 20, 60, 120, \text{ and } 180$ min.

The crystal structure of BaYFeO₄ consists of two crystallographic sites for transition metal ions at the centers of the alternating corner-sharing octahedra Fe³⁺O₆ and square pyramids Fe³⁺O₅, forming Fe₄O₁₈ tetramers. The Rietveld refinement of the XRD data using the previously reported structural model of BaYFeO₄ [2] revealed that our fabricated sample is almost single phase and has the *Pnma* orthorhombic crystal structure with lattice parameters $a = 13.1412(2)$ Å, $b = 5.6938(1)$ Å, and $c = 10.2451(2)$ Å.

At room temperature, the Mössbauer spectra of BaYFeO₄ samples recorded at 4 mm/s and 12 mm/s velocity sweep consists of two doublets D₁ and D₂ with the close values of isomer shift (*IS*) of 0.36 and 0.30 mm/s but with markedly different quadrupole splittings (*QS*) of 0.23 and 0.49 mm/s, respectively, in agreement with our previous work [3]. The first doublet D₁ corresponds to the ferric ions in the octahedral surrounding (Fe^O) and the second doublet D₂ can be attributed to the ferric ions in square pyramids (Fe^{SQ}). In addition to doublets, a sextet corresponding to a small amount of hematite was observed in the Mössbauer spectra of the prepared samples (*IS*=0.43 mm/s, *QS*= -0.41 mm/s, and $B_{\text{hf}}= 50.9$ T).

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MÖSSBAUER SPECTROSCOPY STUDY OF POTENTIALLY MULTIFERROIC BaHoFeO₄

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Multiferroic materials with magnetic, ferroelectric, and/or ferroelastic ordering in specific temperature ranges have drawn significant attention because of the fundamental physical research and their potential applications in emerging fast electronic devices.

A sample of polycrystalline BaHoFeO₄ was prepared by solid-state method. It has an orthorhombic crystal structure with space group *Pnma* (No. 62); $a = 13.13993(1)$ Å, $b = 5.69670(1)$ Å, and $c = 10.24932(1)$ Å at room temperature [1]. Fe³⁺ ions are located in two different crystal environments: FeO₅ square pyramids (site Fe¹) and FeO₆ octahedra (site Fe²). BaHoFeO₄ is isostructural to the well-known BaYFeO₄ compound.

The room temperature transmission Mössbauer spectrum of BaHoFeO₄ consists of two doublets D₁ and D₂ with the close values of Isomer Shift (IS), but with markedly different Quadrupole Splittings (QS). The doublet D₁ corresponds to the ferric ions in the octahedral surrounding (Fe²O₆) and the second doublet D₂ can be attributed to the ferric ions in square pyramids (Fe¹O₅). Furthermore, the Mössbauer spectra of BaHoFeO₄ were collected at low temperatures ranging from 4.2 to 55 K. The paramagnetic doublets remain unchanged until T_{N1} ~ 47 K (in accordance with the data in [1,2]). The magnetic sextets appear in the spectra below T_{N1} as the indication of the onset of the magnetic ordering of iron ions. The spectra between T_{N1} and T_{N2} could be fitted by two sextets with very broad distributions of the hyperfine magnetic fields. This behavior indicates a form of the antiferromagnetic ordering of the iron magnetic moments called incommensurate spin-density waves [2]. Below the transition temperature T_{N2} ~ 37 K [1,2] in a zero external magnetic field, the shapes of the sextet lines are narrowed and well resolved. They could be decomposed into two well-resolved sextets S₁ and S₂ corresponding to the two nonequivalent Fe sites. It is consistent with a commensurate antiferromagnetic structure below T_{N2} [2]. At 4.2 K in a zero external magnetic field, the width of the distribution of the hyperfine magnetic field in sextet S₂ belonging to pyramidal sites increases compared with the value observed at 10 K. The broadening of the lines in the sextet is probably caused by the influence of spontaneous noncollinear ordering of the Ho magnetic moments. In an external magnetic field of 6 T, the antiferromagnetic ordering of magnetic moments in both iron sublattices is probably partially disturbed.

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MULTIFERROIC BaErFeO₄: MÖSSBAUER SPECTROSCOPY STUDY

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Multiferroic materials with magnetic, ferroelectric, and ferroelastic ordering have drawn significant attention from the fundamental physics point of view as well as their potential applications for future electronic devices. A polycrystalline BaErFeO₄ sample was prepared by the conventional solid-state method. It has a unique orthorhombic crystal structure with *Pnma* space group and lattice parameters $a=13.11080(3)$ Å, $b=5.68412(1)$ Å, and $c=10.22506(2)$ Å at room temperature [1]. Fe³⁺ ions are located in two different crystal environments, namely FeO₅ square pyramids (atom Fe^{SQ}) and FeO₆ octahedra (atom Fe^O).

At room temperature, the Mössbauer spectrum of BaErFeO₄ recorded at 4 mm/s velocity sweep consists of two doublets D₁ and D₂ with the close values of isomer shift (*IS*) of 0.37 and 0.30 mm/s but with markedly different quadrupole splittings (*QS*) of 0.25 and 0.50 mm/s, respectively. The first doublet D₁ corresponds to the ferric ions in the octahedral surrounding (Fe^O) and the second doublet D₂ can be attributed to the ferric ions in square pyramids (Fe^{SQ}). Furthermore, the Mössbauer spectra of BaErFeO₄ were collected at low temperatures ranging from 4.2 to 55 K. The paramagnetic doublets remain unchanged until $T_{N1} \sim 49$ K [1, 2], below which the spectra are split into magnetic sextets, indicating the onset of the magnetic ordering of iron ions. The spectrum at 40 K was fitted by two sextets with very broad continuous distributions of the hyperfine magnetic field, indicating an antiferromagnetic ordering of the iron magnetic moments in the form of an incommensurate spin-density wave [2], for which the magnitudes of the iron magnetic moments change dramatically, and so the magnitude of the hyperfine magnetic field too. Below the transition temperature $T_{N2} \sim 34$ K [1, 2], the spectral shapes of Mössbauer spectra acquired at temperatures 30 K, 20 K and 10 K in a zero external magnetic field are narrow and well resolved. They can be decomposed into two well-separated sextets S₁ and S₂, corresponding to the two nonequivalent Fe sites, which is consistent with a commensurate antiferromagnetic structure below T_{N2} [2]. The width of the distribution of the hyperfine magnetic field in the S₂ sextet, belonging to pyramidal sites, increases from the value $\Delta B_{hf} = 0.5$ T observed at 10 K to $\Delta B_{hf} = 1.7$ T at 4.2 K in a zero external magnetic field. The broadening of the lines in the sextet is probably affected by spontaneous noncollinear ordering of the erbium magnetic moments. In an external magnetic field of 6 T, the antiferromagnetic ordering of the magnetic moments in both iron sublattices is disturbed.

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DETERMINATION OF SELECTED ELEMENTS IN CEREAL FLOURS AND THEIR GLUTEN-FREE ALTERNATIVES

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The aim of this study was to provide a basic overview of the elemental composition of gluten-free flours and mixtures, which have not been extensively studied and the results are not widely known. Another objective of this study was to compare this composition with that of flour containing gluten. The study primarily targets people with celiac disease, for whom a gluten-free diet is the only available treatment. It aims to assist individuals in understanding the elemental composition of gluten-free alternatives. The elements selected for determination were those in which a deficiency was assumed due to reduced intake or impaired absorption in individuals with celiac disease. The study primarily focuses on determining the concentration of calcium, magnesium, phosphorus, potassium, sodium, iron, zinc, and copper in cereal gluten flours and their gluten-free alternatives. Individual flour samples were decomposed using a microwave digestion in presence of mineral acids, and the elements in the solutions were subsequently determined using a mass spectrometry with inductively coupled plasma. The result of the study is an overview and comparison of the elemental composition of gluten-containing flours and gluten-free alternatives. This overview can help people with celiac disease in selecting suitable gluten-free alternatives and serve as a guide for mixing flours to enrich dishes with the necessary elements.

MÖSSBAUER STUDY OF SURFACE CHARACTERISTIC OF 316L STAINLESS STEEL AFTER TEMPERATURE IMPACT IN OXIDIZING AND INERT ATMOSPHERES

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The method of Mössbauer spectroscopy can be used for studying the surface layer and the bulk of the material. For volume investigation of the material is appropriate Conversion X-ray Mössbauer spectroscopy (CXMS), which gives information about structure in depth of 10 μm . In the case of surface layer examination, Conversion Electron Mössbauer Spectroscopy (CEMS) is appropriate technique due to the fact that the penetration depth of conversion electrons is approximately 0.3 μm . The combination of both ways is allow to obtain the information about inhomogeneity of the specimen.

Austenitic stainless steel has corrosion resistant protective layer. The main component of this layer is chromium oxide (Cr_2O_3), which is the result of the reaction with oxygen contained in the air. Investigated samples were made from metallic powder of austenitic stainless steel 316L by selective laser melting (Concept Laser, Germany). The finished samples have the shape of plates with the size 25x25x2 mm^3 . After manufacturing, specimens were sandblasted by corundum powder. After the polishing samples were annealed in air and another part was kept in argon atmosphere. The annealing temperature for all samples was 550 $^\circ\text{C}$ and duration of time was 0.5, 1, 2, 16 hours. The samples that were kept in an inert atmosphere were also under pressure in 0, 0.6, 1, 2 atm. In addition to Mössbauer spectroscopy, scanning electron microscopy (SEM), energy-dispersive analysis (EDS), X-ray diffraction (XRD) and positron annihilation methods were chosen for surface investigation.

According to CXMS results, all spectra show the presence of traditional FCC austenite (γ - phase). It leads to the conclusion that on the depth approx. 10 μm temperature and atmosphere have no impact on the phase change. Based on CEMS spectra were observed that on the thin surface layer after annealing in air appeared spinel type oxide $(\text{Fe-Cr})_2\text{O}_3$. In the case of an inert atmosphere, surface oxidation is also observed during argon annealing. This effect can be explained by the fact that unannealed sample before temperature and atmosphere influence, have very thin oxide layer on the top mainly containing chromium.

REAL-TIME OBSERVATIONS OF ACETAMINOPHEN'S TRANSFORMATIONS FOLLOWED BY ADVANCED TECHNIQUES OF RAMAN SPECTROSCOPY

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The technique of surface-enhanced Raman scattering (SERS) which is known for 50 years offers many advantages. Nevertheless, the proper interpretation of SERS spectra remains a challenging aspect to overcome, especially when encountering some of the special cases. The aspects include the various effects of chemical enhancement, which could be a possible result of transformation of chemical species induced by the interaction with incident radiation. Although such behavior was reported several times, the variety of molecules undergoing such transformation seems to be almost uncountable and contains also some medicinally important molecules. [1, 2]

Here, we report the observation of photochemical reactions of acetaminophen, adsorbed on the Ag, Au and Cu enhancing substrates. Using several excitation wavelengths from the visible (457, 532, 633 nm) and near infra-red spectral region (785 and 1064 nm), we were able to dive deep into the described problematics, unveiling a strong tendency of acetaminophen to transform due to the incidental radiation. From the various sequential measurements, we were able to record multiple possible pathways, which can be undergone by the adsorbed molecules of acetaminophen. Such results were confronted with the DFT calculations, which prove themselves useful for the explanation of at least some of the recorded effects.

As the acetaminophen is medicinally important molecule, we believe that presented findings could be applied to its proper SERS spectrochemical analysis. Nevertheless, our results could bring enlightenment to some of the questions arising from the mentioned field, making presented results part of the larger field of plasmon-assisted photochemistry.

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BIOIMAGING OF PLANT MATERIALS USING LA-ICP-MS

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Industrialization and urbanization have induced the accumulation of toxic substances in soil, water and air, prompting the need for sustainable remediation approaches like phytoremediation. This technology involves the use of green plants to degrade, fix, or accumulate various pollutants. The branch of this method, phytoextraction, represents a method in which plants accumulate contaminants, which are then harvested and processed (e.g., thermally, microbially, or chemically). This process primarily removes metals, but it can also be used to remove metalloids, radionuclides, or non-metals. Phytoextraction is primarily used to clean contaminated soils. ^[1]

In this experiment, an analysis of the lentil plants was carried out, which was treated with foliar application of gold nanoparticles (Au NPs). It has been proven that Au NPs can be used as nanofertilizers, which improve the effectiveness of the plant's phytoremedial capabilities. The accumulation and distribution of Au in the leaves of this plant were compared in relation to the period to which they were exposed. Lentil leaves treated with only water served as a control. The analysis of the lentil leaves was performed using the laser ablation method combined with inductively coupled plasma mass spectrometry (LA-ICP-MS).

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STUDY OF THE HOMOGENEITY OF SILICA GLASS

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A series of model glasses with silicate matrix $\text{SiO}_2\text{-Na}_2\text{O-CaO-Al}_2\text{O}_3\text{-K}_2\text{O}$ was prepared. Glass batches were melted at different time intervals of 4, 5, 6, and 7 hours in an elevator furnace and ambient atmosphere [1]. The composition of the prepared glasses was determined by X-ray fluorescence elemental analysis (XRF Tiger, Bruker) [2], and an optical emission spectrometer with inductively coupled plasma (ICP-OES 5100SVDV, Agilent) [3] after microwave digestion.

Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS, LSX-213 G2+, Teledyne) [4] was used to study the homogeneity of model glasses. Lateral and in-depth spot and line analysis were performed. Relative standard deviations (% RSD) of the isotopes were calculated from the measured intensities values. Material with an RSD value < 5% of the measured isotopes was considered to be homogeneous [4].

Laser ablation revealed homogeneity differences between samples melted for 4 (~ 10 % RSD) and 5 (~ 5 - 7 % RSD) hours. The difference between the samples melted for 5, 6, and 7 hours was negligible. The reproducibility of the results was confirmed by repeating the melting experiment and evaluating the same process (~ 5 - 7 % RSD).

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STUDY AND INTERPRETATION OF CORROSION PRODUCTS OF FIBERGLASS INSULATION BY RAMAN SPECTROSCOPY

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In nuclear power plants, corrosion is an undesirable phenomenon, especially in connection with Loss of Coolant Accidents (LOCA) [1]. The chemical composition of fiberglass insulation and glass grains was determined using X-ray Fluorescence (XRF) analysis. Static and dynamic leaching experiments were carried out at different temperatures for 30 days. Distilled water and borate solution of Na₂B₄O₇/H₃BO₃ coolant with pH 8.6 were used as corrosion medium [2]. The surface changes in corroded samples were observed using scanning electron microscopy (SEM/EDS) (Fig. 1). Additionally, the corrosion products were identified using Raman spectroscopy (Fig. 2). The following corrosion products were detected: Pyrophyllite / Al₂Si₄O₁₀(OH)₂, Tridymite / SiO₂, K-Mica / KAl₃Si₃O₁₀(OH)₂, Calcite / CaCO₃.

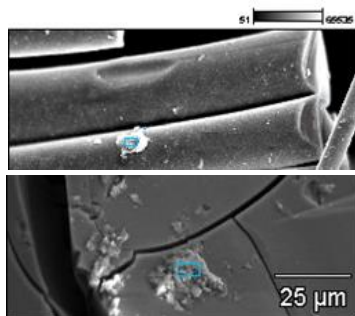


Fig 1. SEM images of corroded fiberglass, and glass grains.

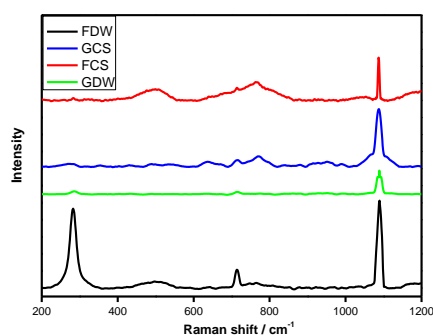


Fig 2. Raman spectra of fiberglass and glass grains corroded in distilled water and in coolant solution

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RAMAN SPECTROSCOPY STUDIES OF VARIOUS MODEL SILICA GLASS FOR MEDICAL GLASS APPLICATIONS

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The syntheses of model silica glass compositions based on medical glass have been realized via the standard melt-quench method. The base glass composition was modified by varying the oxide content. Basic physicochemical properties such as viscosity, density, glass transition temperature, and thermal expansion were characterized. The major oxide/element composition of prepared glass batches was determined by X-ray fluorescence elemental analysis (XRF).

The structure of prepared glasses was analyzed by Raman spectroscopy. The following Raman bands were detected in the spectrum of prepared glasses (Fig. 1.): the most intense and narrow band with a maximum near 500 cm^{-1} attributed to the mix stretching and bending of Si-O-Si units, the less strong narrow band at about 650 cm^{-1} , two broad peaks at about 700 and 800 cm^{-1} , two broad and weak bands with the maximum of about 920 cm^{-1} and 1300 cm^{-1} , and the medium intense and broadband with the maximum peak at 1050 cm^{-1} . The peaks in the region between 850 to 1250 cm^{-1} indicate the stretching of the Si-O bond within silicate tetrahedra. A similar structure was also observed in other varieties of studied model glasses.

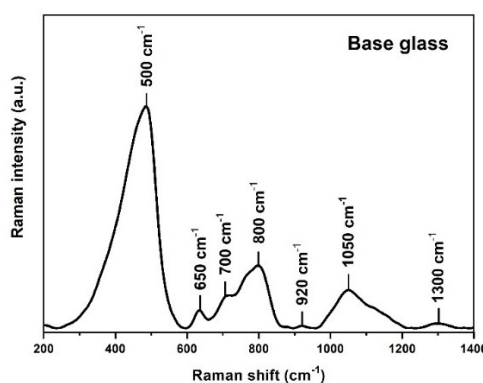


Fig. 1. Raman spectrum collected from the base model silica glass.

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THE MECHANISM OF INTERACTION OF G-QUADRUPLEXES WITH THE PLANT ALKALOID FAGARONINE

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Fagaronine is a plant alkaloid from the group of benzophenanthridine alkaloids, which is commonly found in the roots of the *Fagara zanthoxyloides* plant. Several benzo[c]phenanthridine alkaloids have already been shown to have a stabilizing effect on non-canonical structures, in particular on G-quadruplexes, which are secondary DNA structures occurring on guanine-rich sequences, especially at the ends of telomeres. Increasing the stabilization of these structures can inhibit DNA replication or transcription, which can result in a significant reduction in cell division.

Since the stabilizing effects of fagaronine on G-quadruplex structures have already been demonstrated, I am focusing this work on a more detailed study of the interaction mechanism to better understand the alkaloid's stabilizing influence. A series of experiments, including NMR spectroscopy, have been carried out with three types of G-quadruplexes (parallel, antiparallel, hybrid).

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MODIFICATION OF CHEMILUMINESCENCE SYSTEM FOR BLOOD SPOT DETECTION

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The work focused on improving the luminol chemiluminescence system, often used in forensic science to detect blood spots. In the experimental part, the emission parameters of various modified luminol systems were investigated. These results were used to optimize the chemiluminescence conditions of the luminol mixture. Identical measurements were also performed on Bluestar tablets, which are now the established standard for blood spot detection. The results obtained led to the design of an optimal system for chemiluminescence detection of blood spots. As part of the effort to improve the system, the CRET (Chemiluminescent Resonance Energy Transfer) method was investigated on fluorescent substances (fluorescein, eosin, rhodamine 6G, rhodamine B and rhodamine 110) as a potential means to increase sensitivity and detection efficiency. In addition, efforts were made to prevent luminescence quenching due to the substitution of solvent (H₂O) for deuterated water (D₂O). The proposed improvements were subsequently tested and compared on synthetic blood spots.

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INVESTIGATION OF DEFECTS IN 2D MATERIALS USING RAMAN SPECTROSCOPY

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Two-dimensional (2D) materials are a class of materials with exceptional properties due to their unique structure. They typically consist of one individual layer with a thickness on the atomic level. In recent years, they have gained considerable attention thanks to their exclusive properties and the associated almost unlimited application potential, for example in nanotechnology, electronics, sensor technology and energy storage. The structure of 2D materials are often presented as an ideal crystal with no imperfections, however presence of defects is inevitable and defects can play a significant role for the performance of any device [1,2]. Thus, in certain cases the presence of a specific type of defect is desirable to achieve certain specific capabilities of a 2D material, a branch of materials research commonly referred to as intentionally induced defect engineering [1].

Raman spectroscopy emerges as a powerful tool for probing and characterizing defects in 2D materials. By analyzing the vibrational modes of the material, Raman spectroscopy provides valuable insights into the presence and nature of defects, offering a non-destructive and sensitive means of defect detection [3]. One possible procedure for creating defects is to expose the 2D material to ion beam or plasma in ultra-high vacuum (UHV) environment, which ensures minimal interference from impurities and provides an ideal platform for precise control of experimental conditions. Since defects in graphene are well-known described by Raman spectroscopy we used it as a probe for investigating defects in MoS₂. We exposed both materials to the same doses of ions and we study in detail effect of increasing number of defects on Raman features of both materials.

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MULTIVARIATE OPTIMIZATION OF THE FEATHER SAMPLE CLEANING PROCEDURE PRIOR TO ICP-MS ANALYSIS

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This study aimed to develop an effective washing procedure for feather samples prior to multi-element ICP-MS analysis. Various washing schemes, were tested using different cleaning solutions, including deionized water with detergent, ethanol, acetone, nitric acid, ethylenediaminetetraacetic acid tetrasodium salt (EDTA), and citric acid (CA). For this purpose, a multivariate design was employed, allowing for optimization in a short period, generation of a large amount of information from a small number of experiments, and the evaluation of the interaction between variables. Specifically, a two-level fractional factorial design with central points was utilized to identify critical factors and their optimal levels, such as concentrations, volumes of analytical agents, and extraction time using ultrasonication. The optimized cleaning procedure involved sequential use of deionized water with detergent followed by a mixture of acetone, EDTA, and diluted nitric acid with sonication, which yielded the best results for multianalyte ICP-MS analysis. This method was successfully applied to analyze certified reference materials for human hair (GBW07601 and NCS ZC 81002b) and various feather samples collected from polluted and control locations in Slovakia, demonstrating its efficacy in determining metal load. The integration of multivariate statistical analysis in this context proved invaluable for understanding the effects of pollution on the elemental profiles of samples in different environmental settings.

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MULTIMODAL CORRELATIVE IMAGING OF HUMAN TOOTH ANKYLOSIS

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Human tooth ankylosis is a pathological condition that manifests as a firm junction of the tooth root and surrounding alveolar bone. The causes of its origin on the molecular levels are still rather uncertain, the main working hypothesis describing its development as a result of damage in the cementum layer, followed by bone cells binding in that area [1].

Therefore, in this study, we propose a correlative imaging approach for a complex characterization of human tooth ankylosis. To achieve that, we implemented a combination of methods Laser-Induced Breakdown Spectroscopy (LIBS), Micro-Computed Tomography (μ CT), Raman spectroscopy, and Histology. Firstly, before the sample preparation, μ CT was used to precisely localize the ankylotic area. Subsequently, the elemental changes associated with the ankylosis development were investigated by the rest of the mentioned techniques. Correlation of these results provided a detailed characterization of this pathology, showing a significant elemental disbalance in the ankylotic area.

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INVESTIGATING BIOINDICATOR ELEMENT DISTRIBUTION IN VARIED SKIN TUMORS VIA CORRELATIVE IMAGING

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Integrated imaging techniques for evaluating cutaneous tumors offer supplementary knowledge to conventional histopathological examination. However, the extensive clinical use of advanced analytical methods such as Laser-induced breakdown spectroscopy (LIBS) and Laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) is still limited. LIBS is a sufficient pre-screening method for large sample sets according to the speed and reproducibility. In contrast, LA-ICP-MS is a ground truth and reference technique for preselected samples. This research highlights the benefits of combining these modalities, which can provide complementary data concerning major biotic (Ca, Mg, P) and trace (Cu, Zn) elements within tumor tissues [1].

The investigation focused on determining changes in elemental distribution in various tumors, including malignancies (squamous cell carcinoma, basal cell carcinoma, malignant melanoma, and epithelioid angiosarcoma), one benign pigmented nevus, and one sample of healthy skin. The data processing was based on a methodological pipeline involving binary image registration and affine transformation. This work brings a feasibility study of a practical methodological concept that enables comparing LIBS and LA-ICP-MS results despite the mutual spatial distortion of original elemental images.

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EXPLORING THE ELEMENTAL COMPOSITION OF DIFFERENTLY AGED MICROPLASTICS: INSIGHTS FROM LASER-INDUCED BREAKDOWN SPECTROSCOPY AND RAMAN SPECTROSCOPY

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Microplastics, small plastic particles resulting from the degradation of larger pieces of plastic, pose an environmental threat due to their persistence, accumulation in ecosystems and potential harm to human health [1]. Laser-induced breakdown spectroscopy (LIBS) is a technique that employs laser source to create plasma plume and reveals the elemental composition of samples by analysing the emitted light [2]. On the other hand, Raman spectroscopy detects energy changes in scattered light caused by molecular vibrations [3].

This poster presents the results of our study, in which we used LIBS and Raman spectroscopy to investigate the elemental composition of different microplastics and their aging process. Our meticulous analysis revealed distinct elemental signatures for each type of microplastic, significantly improving our ability to identify and characterise these pollutants. This could contribute to a better understanding of microplastic pollution.

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ANALYSIS OF MACROBIOGENIC ELEMENTS IN QUALITY WINES FROM SELECTED PRODUCERS USING THE AAS METHOD

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Two macrobiogenic elements (Ca and Mg) were determined in the samples of branded varietal wines by the AAS method in order to analyze the possible way of entry of these monitored elements into alcoholic beverages. This analytical method was used to determine the presence of these metals in four varietal wines from five producers in order to determine the dependence of these element contents in drinks on the locality (the influence of the soil type was assessed) or on the influence of the human factor (assessment of the method of production technology of these wines).

The calcium values ranged from 42.0 to 72.6 mg.kg⁻³, while the highest value was recorded in the Chardonnay variety from the producer Vinárstvo Tajna, and the lowest was also in the same variety, which came from the Vinárstvo Predium, and the magnesium values ranged from interval 44.3 – 123.4 mg.kg⁻³, while the highest value of this element was recorded in the variety Frankovka modrá from the producer Vinárstvo Predium, and the lowest was in the variety Chardonnay, which came from the producer Pivnica Tibava.

After averaging all values of calcium amounts in varieties from individual producers, the following order of average values of this element in four varietal wines produced by producers was found: Vinárstvo Tajna > Vinárstvo Movino > Pivnica Tibava > Vinárstvo Elesko > Vinárstvo Predium and this order of average values of magnesium in four varietal wines from producers: Vinárstvo Predium > Vinárstvo Tajna > Vinárstvo Movino > Vinárstvo Elesko > Pivnica Tibava.

The contents of these two investigated elements in all varieties from the given wine producers were also further averaged and the following order of varieties in terms of calcium was obtained: Rízling Rýnsky > Chardonnay > Frankovka modrá > Pálava. The order of average magnesium values in varietal wines was as follows: Frankovka modrá > Pálava > Rízling Rýnsky > Chardonnay.

From the resulting analyzes obtained, a greater influence of the locality of individual producers and their method of wine can be observed, compared to the contents of these two macrobiogenic elements, than the varieties used for the production of these alcoholic beverages. Therefore, it would be possible to determine the so-called "a elemental key" that would characterize the composition of wines from individual producers.

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NEW GLASS CALIBRATION STANDARDS FOR LA-ICP-MS: DEVELOPMENT, TESTING AND APPLICABILITY

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Mineral resources are used as energy sources and often serve as the basis for the development of new technologies. The determination of the chemical composition of these materials is important for the applicability, treatment, and exploration of deposits. One of the methods used for the analysis of geological materials is Laser Ablation Inductively Coupled Plasma Mass Spectrometry (LA-ICP-MS). Despite the wide range of applications of this method, accurate determination of elemental content due to matrix effects and elemental fractionation remains one of the major challenges. For quantification, an external calibration standard is most commonly used, but the number of commercially available standards is very limited, and the preparation of in-house standards is complicated by the requirement of homogeneity and well-defined composition¹. Therefore, there is an effort to develop new calibration standards with different analyte compositions than those provided by commonly available standard reference materials.

The aim of this study was to create new calibration standards for quantification of elemental contents, especially of geological samples in the field of strategic mineral technology research. The glass samples were supplied by FunGLASS (Centre for Functional and Surface Functionalised Glass). The elemental homogeneity of the newly prepared glasses was tested by the LA-ICP-MS method. The first step was a test of the base glass, which consists of matrix elements. A series of model glasses with silicate matrix SiO₂-Na₂O-CaO-Al₂O₃-K₂O was prepared. Glass batches were melted at different time intervals of 4, 5, 6, and 7 hours to optimize the melting time. Homogeneity was investigated both by LA-ICP-MS spot analysis and subsequent RSD calculation, and by measuring elemental distribution maps for graphical description of homogeneity. The subject of further research is the preparation of glasses containing elements of interest in the given contents and the subsequent homogeneity testing.

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SEPARATION OF SELECTED ELEMENTS FROM THE SAMPLE MATRIX FOR ICP-MS USING COMMERCIAL AND "IN-HOUSE" PROCEDURES

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This work aims on utilizing laboratory synthesized monolithic stationary phase for the separation of selected elements (U, Th, Pb, Sr) with potential application in isotope analysis, which is widely used in several fields, including archaeology [1], geochemistry (Pb-Pb and U-Pb dating) [2] or food technology [3]. Most applications require separation of the monitored elements from the matrix prior analysis itself, either due to interferences (^{87}Rb and ^{87}Sr) or preconcentration of the analyte. The design of the separation controls resulting accuracy of the analysis and in some cases allows experiment to be performed at all.

Currently, the separation is performed with commercially available columns and ion exchangers, e.g. Amberlite® IR-120 (strongly acidic cation exchanger, H^+ form; supplier: Merck KGaA Germany), which significantly increase the overall cost of the analysis. The utilization of columns with a monolithic stationary phase is an interesting alternative. Monolithic stationary phases find applications in several different separation problems such as the separation of low molecular analytes [4] or peptides [5]. The main advantage is tailored preparation of separation columns with desired properties. Hence, this work focuses on the specific preparation of polymer-based stationary phases based on vinylphosphonic acid monomer possibly applicable in the isotope analysis of selected elements.

After the separation of model samples consisting of mixture of reference materials (U, Th, Pb, Sr) in 0,01M hydrochloric acid on the prepared columns, individual fractions are analyzed by inductively coupled plasma-quadrupole mass spectrometer (ICP-QMS). Hydrochloric acid of different ionic strengths, carbonate buffer and MQ water are used as elution reagents. Separation parameters (e.g. flow rate, volume of fractions etc.) were optimized over time. Emphasis is placed on both qualitative and quantitative analysis. The complexity of the process, quality of the separation as well as cost of procedure are evaluated.

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STUDY OF CARDIAC REMODELLING BY LA-ICP-MS

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Laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) is one of the most important analytical techniques used in trace analysis. High sensitivity and accuracy, low detection limits and the ability to directly analyse solid materials allows the employment of the method in bioimaging. Determination of elemental distribution is convenient in medicine, in order to understand the development of various diseases, to improve diagnostic methods, therapy or to track metalloproteins. Investigation of cardiovascular diseases are the leading cause of death globally, may be one application. Cardiac remodelling and myocardial fibrosis are closely related to heart failure and no effective medical care exists for both diseases. Therefore, prediction and related better diagnosis is crucial. LA-ICP-MS provides the investigation and 2D-imaging of metals included in metalloproteins, which have a major role in tissue remodelling.

In this experiment, samples of rat heart sections with induced cardiac damage and remodelling were analysed by LA-ICP-MS. The aim of the work was to focus on the elemental distribution related to the enzymes and proteins located in the damaged tissue and to find out the indicator of damaged tissue early before the remodelling process occurs.

Acknowledgements

The work was supported by the project FCH-S-24-8591 of Ministry of Education, Youth and Sports of the Czech Republic.

ANALYTICAL METHODS FOR MONITORING THE EFFICIENCY OF DECOMPOSITION OF GADOLINIUM-BASED CONTRAST AGENTS

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In the last 40 years, there has been a considerable technological progress in the field of medical imaging techniques. Magnetic resonance imaging (MRI) is an effective tool for the early diagnosis of various diseases. Using specific, paramagnetic properties of gadolinium, the effectiveness of MRI diagnostics has become higher due to gadolinium-based contrast agents (GBCA). In the last 30 years, their considerable expansion has led to an increase in anthropogenic pollution of the environment with this metal from the urine of patients or the residual unused amount, which could be recycled and reused using modern waste management methods [1, 2].

The goal of the work was to design and optimize the recycling process of residual GBCA material together with packaging materials (glass, plastic, aluminum, rubber, adhesives) that are incinerated in hospital incinerators. The acid decomposition of GBCA using microwave radiation was tested, with the resulting product being a gadolinium salt (gadolinium nitrate). Three parameters were optimized during the decomposition process, namely the amount of decomposition agent (nitric acid), the time program and the temperature program. The efficiency of contrast agent degradation was based on monitoring the concentration of gadolinium and residual organic carbon in the mineralized using inductively coupled plasma optical emission spectrometry (ICP OES) and total organic carbon (TOC). By optimizing the microwave decomposition parameters, almost 100% decomposition effectiveness was achieved, and gadolinium was obtained in the aqueous (gadolinium nitrate). Microwave-assisted acid decomposition has been found to be an effective method of recycling gadolinium in the form of an inorganic salt, which is the main output of rare earth metal mining. This strategy can create a potentially new source of gadolinium, either for medical purposes or for use in energy and other sectors of industry.

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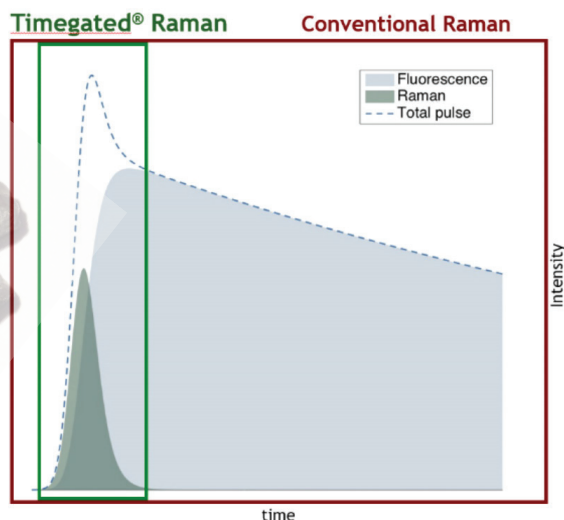
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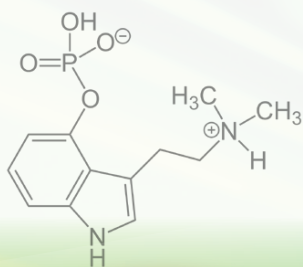
Ramanova spektroskopie je velmi silný nástroj každé moderní laboratoře. Je to rychlá, spolehlivá, jednoduchá a relativně levná analytická metoda, která nevyžaduje hluboké znalosti ani složitou přípravu vzorku. Během několika desítek vteřin poskytuje detailní informace o chemickém složení vzorku, jeho krystalické struktuře i fyzikálních vlastnostech. Je možné s ní měřit mikroskopické vzorky i rozměrné objekty, a Ramanova spektra lze měřit dokonce i přes řadu obalových materiálů. Na problémy ovšem naráží v případě fluorescence, která může některá měření zkomplikovat, nebo i zcela znemožnit, což je časté např. u vzorků biologického původu či barevných materiálů. Existuje řada způsobů, jak s fluorescencí bojovat, z nichž každý má své výhody i nevýhody. Společnost Timegate však jako první na světě nabízí integrovaný systém s jedinečným řešením **reálného potlačení fluorescence**, a tak je s jejími spektrometry možné měřit i vzorky, jejichž analýza s běžnými spektrometry nebyla možná.

Jedinečný spektrometr **PicoRaman M3** můžete mít v sestavě s mikroskopem pro měření všech typů mikroskopických vzorků, celou pro eliminaci odraženého záření či sondou pro vzorky jako např. umělecké předměty, archeologické vzorky a další. Jelikož měří zároveň Ramanovo spektrum i fluorescenci, poskytuje jedním měřením celou řadu zajímavých a důležitých informací.

Své uplatnění tak nachází v geovědách, biofarmaceutickém a forenzním výzkumu, ve farmacii, výzkumu katalýzy a mnohých dalších oborech.



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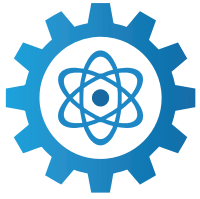
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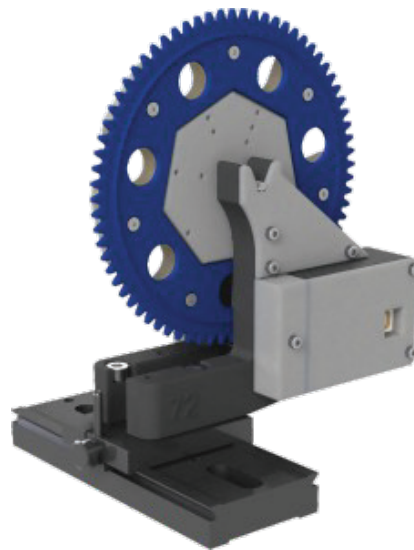
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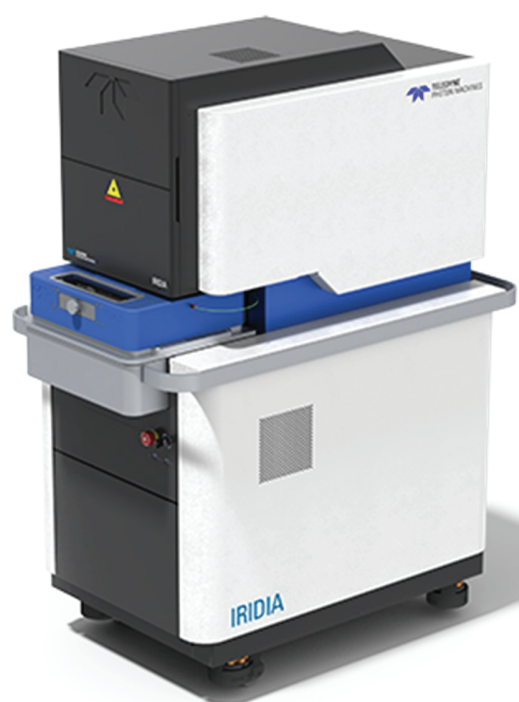


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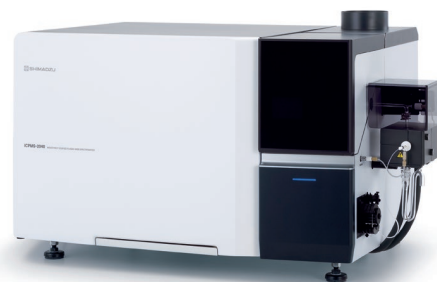
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