

# Book of Abstracts

## INTERM 2024



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11<sup>th</sup> International Congress on Microscopy & Spectroscopy

**11<sup>th</sup> INTERNATIONAL CONGRESS ON  
MICROSCOPY & SPECTROSCOPY  
(INTERM 2024)**

**Oludeniz, Turkey**

**APRIL 18-24, 2024**

## 11<sup>th</sup> International Congress on Microscopy & Spectroscopy

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**PLENARY SPEAKER**

**Id-713**

**3D Imaging and Spectroscopy of Complex Biological Systems at the Sub-Cellular,  
Cellular and Multicellular Levels**

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**Abstract:** The non-invasive nature of optical microscopy enables us to study a great variety of materials under conditions approaching or similar to their "natural" environment. This is especially relevant to live biological specimens, which can be studied both in-vitro and in-vivo, providing a unique insight into the dynamic processes occurring in the live organisms. In recent years, the emphasis has been shifting towards the technologies that combine several different techniques to study a particular biological system, which in turn allows measuring a partially overlapping set of parameters, leading to deeper understanding of processes occurring within that system. In this presentation, I will consider the applications of phase imaging techniques, namely Digital Holographic Microscopy (DHM) and Transport of Intensity Equation (TIE), together with fluorescent and Raman spectroscopic imaging to cellular apoptosis, neurocognitive disorders, mapping of intracellular iron and ferroptosis. Methods of tracking morphological cell changes are based on measurements of phase, which is proportional to the cell thickness and can be extended to measure the optical path length, and, therefore, cell volume. Additionally, Raman micro-spectroscopy is widely used for the mapping of chemical composition within live biological samples, such as cells, organoids, and tissues. It permits non-invasive and non-destructive measurements that do not require special sample preparation processes, such as dye labelling or staining. Another form of programmed cell death, ferroptosis, is the main cause of tissue damage driven by iron overload and lipid peroxidation. Currently, only invasive cell biological assays are used to monitor the expression level and subcellular location of proteins that are known to bind iron or be involved in ferroptosis. Our group has previously reported a Raman spectroscopic method to visualize and quantify the distribution of multiple iron-binding proteins in intact cells and tissues.

**Keywords:** Quantitative Phase, Phase Imaging, Digital Holography, Transport of Intensity Equation, Raman Hyperspectral Imaging, Fluorescence



**PLENARY SPEAKER**

**Id-716**

**Probing the Intermolecular Vibrations and Reorientation in Liquids and Solutions  
by Femtosecond Raman-Induced Kerr Effect Spectroscopy**

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**Abstract:** The intermolecular dynamics in liquids and solutions includes the intermolecular vibrations and reorientations. These molecular motions influence or even control the elementary reaction processes in solution. Therefore, the intermolecular dynamics of liquids and solutions is a very important basic theme in chemistry. The intermolecular dynamics in liquids and solutions occurs in the time scale from tens of femtoseconds (fs) to hundreds of picoseconds (about  $10^3$  to  $10^{-1}$  cm<sup>-1</sup> in the frequency scale with the wave number unit) depending on the target system. Thus, studying the molecular motions in the low-frequency region (approximately 200 cm<sup>-1</sup> or less) is essential for a detailed understanding of the intermolecular vibrations and reorientations in liquids and solutions. Femtosecond Raman-induced Kerr effect spectroscopy (fs-RIKES) is a third-order nonlinear spectroscopy that detects the molecular motions of condensed phases in the low-frequency region (typically ca. 1 – 500 cm<sup>-1</sup> or ca. 0.3 – 15 THz) without the contribution of Rayleigh scattering. In this talk, I will give a talk about some examples of our studies of the low-frequency intermolecular dynamics in liquids and solutions by fs-RIKES, as well as some essences of fs-RIKES technique. They might include simple aprotic molecular liquids, ionic liquids, polymer solutions, bio-related molecules, etc.

**Acknowledgement:** The works discussed in this talk were supported in part by JSPS KAKENHI (JP19K05382, JP22H02028, and JP22H04520).

**PLENARY SPEAKER**

**Id-734**

**Seeing Matter from Ultra-small to Ultra-fast and to Ultra-cold with Electrons**

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**Abstract:** One of the grand challenges in modern science and engineering is the ability to directly observe materials' behavior in ultimate space (the ultra-small world) and time (the ultra-fast world). While the ultra-fast can unravel how the fundamental building blocks of matter respond to applied stimulus, the ultra-small may allow us someday to design and assemble novel energy materials at atomic level. Furthermore, in many areas of condensed matter physics and materials science, the ability to observe atomic and electronic structures at ultra-cold environment is extremely important as many intriguing physical phenomena occur at extremely low temperatures. In this presentation, I will give a brief overview of our recent work on the study of charge-orbital-lattice interplay in quantum materials and ionic transport in energy storage materials using state-of-the-art electron microscopy that is barely matched by any other methods. Three examples will be given: 1) The development of atomically resolved in-situ biasing experiments using aberration corrected transmission electron microscopes to directly observe the role of defects in Li-ion diffusion in low-dimensional battery electrodes; 2) The development of 2.8MeV-130fs ultrafast electron diffraction system that enables us to reveal lattice dynamics, competing orders of electrons and phonons, and hidden states far-from equilibrium to address some key issues in strongly correlated electron systems; and 3) the development of atomically resolved scanning transmission electron microscopy (STEM) and electron energy-loss spectroscopy (EELS) at liquid-He temperature (<10K) to study interfacial two-dimensional electron gas and charge transfer across a monolayer FeSe films grown on SrTiO<sub>3</sub> substrate. The approach allows us to directly observe interfacial atomic arrangement and valence states above and below superconducting critical temperature and compare the results with electric backgating measurement and Roman spectroscopy to understand the origin of the 10-fold enhanced superconductivity at the interfaces. If time allowed, I will also report our recent electromagnetic biasing experiments at low temperatures (10-20K) on chiral spin texture materials that have a non-trivial topology to reveal the transitions mechanism of helical and skyrmion phases using a quantitative phase-retrieval method we developed recently.

**Keywords:** high-resolution STEM, in-situ electron microscopy, ultrafast electron diffraction, electron energy loss spectroscopy, Lorentz microscopy

**Acknowledgement:** The author would like to acknowledge the electron microscopy group at BNL for assistance. The work presented was mainly supported by the US DOE/BES-MSD under Contract DE-SC0012704.

PLENARY SPEAKER

Id-752

**Confocal Microscopy Imaging of *Drosophila Melanogaster* Embryos Exposed to Tumour Treating Alternating Current Electric Fields**

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**Abstract:** Brain and nervous system cancers killed over a quarter of a million people globally in 2020<sup>(1)</sup>. Of this category of cancers, Glioblastoma is the most common primary malignant brain and central nervous system tumour in adults. The current standard of care for the treatment of GBM is surgical resection followed by concomitant treatment with radiotherapy and the chemotherapy drug Temozolomide (TMZ)<sup>(2)</sup>. Throughout their treatment patients often report low quality of life partly caused by treatment side effects which can include, nausea, fatigue and joint pain. Despite intensive treatment, the median survival for Glioblastoma patients is only 15 months. Evidently, there is a clear need to develop effective treatments with reduced side effects compared to the current standard of care. The need for novel Glioblastoma therapies has led to the development of Tumour Treating Field (TTF) therapy. TTF therapy is a FDA approved innovative treatment method that uses low intensity (1-3V/cm), intermediate frequency (150-250kHz) electric fields to treat Glioblastoma. The electric fields exert a range of anti-cancer effects on rapidly proliferating cells such as interference with tubulin polymerisation during metaphase and increasing cell membrane permeability<sup>(3)</sup>. Currently, the only approved TTF therapy device is Optune™ developed by Novocure. The Optune™ TTF treatment system delivers TTF fields to the tumour site through the skin and scalp via adhesive pads which contain electrodes connected to a lightweight portable battery. Critically, the only reported side effect of this treatment is mild skin irritation caused by the adhesive at the electrode attachment site. As the device is portable, patients can receive TTF therapy outside of a clinical setting contributing to a higher quality of life compared to conventional treatment modalities. Whilst originally developed for the treatment of Glioblastoma, several clinical trials and studies investigating the efficacy of this treatment for other solid tumour types such as lung<sup>(4)</sup> and breast<sup>(5)</sup> are ongoing. Whilst TTF therapy has been demonstrated to increase the overall survival of Glioblastoma patients, the therapy is currently only approved whilst in combination with a TMZ chemotherapy regime. The ultimate aim of this study is to improve the efficacy of TTF treatment, so that TMZ may not be needed as an adjunctive therapy to TTF. In this study we used transgenic *Drosophila melanogaster* embryos as a model organism for studying the anti-cancer effects of TTF *in vivo* and in investigating optimal TTF parameters (frequency and voltage intensity). *Drosophila* is an appropriate model to use as mitotic processes are conserved to that of humans and in the

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early embryo, cell divisions occur rapidly. Using live confocal microscopy we identified abnormal mitotic phenotypes that are induced by application of TTF. The induced phenotypes appear to prevent further development and may lead to cell death. Additionally, the effect of TTF on the nervous system was investigated. We found that TTF may cause a change in the rate of muscle contraction but that this effect appears to be reversible upon field removal. Future work will include the application of TTF optimised in *Drosophila* to a cultured human Glioma cell line, the investigation of TTF on live firing in *Drosophila* neurons and the application of TTF to a *Drosophila* brain tumour model.

**Keywords:** Tumour Treating Fields, Glioblastoma, *Drosophila Melanogaster*

**PLENARY SPEAKER**

**Id-759**

**Interconnection of Microscopy and Radiology in Medical Imaging**

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**Abstract:** Medical imaging traditionally refers to mostly radiology, noninvasive macroscopic imaging of the human body, including ultrasound, x-ray radiography, computed tomography, and magnetic resonance imaging (MRI). Medical microscopy or pathology of tissue samples from patients should also be regarded as part of medical imaging. Radiological imaging is limited in molecular specificity as a voxel contains millions of molecules, and pathologic imaging is limited by tissue sampling as biopsy is a hit-miss. Accurate disease assessment in medicine requires synergistically combining noninvasive volumetric coverage of radiology with invasive molecular specificity of pathology. Traditional interconnection of pathology and radiology includes biopsy guidance by radiological imaging, and radiologic image feature interpretation based on pathology. Modern computing power and artificial intelligence are enabling exciting new developments for connecting pathology and radiology. Radiomics, pathomics and genomics are integrated into multiomics for accurate disease progression. Multiscale biophysics modeling allows microscopic inference in noninvasive radiology. This exciting new development of pathology, radiology and machine learning will be exemplified in multiscale physics learned magnetic resonance imaging.

**Keywords:** Radiology, Pathology, Multiscale Physics, Magnetic Resonance Imaging

**PLENARY SPEAKER**

**Id-762**

**Structure-Function Correlation in Advanced Materials Using Synchrotron Based Spectroscopy**

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**Abstract:** In this talk I will do a review of structure and device function correlations of several advanced material systems in semiconductor industry using synchrotron radiation-based spectroscopies. Material based problems of semiconductor-based devices can best be resolved with the detailed structural information and the correlation between the introduced subtle structural changes and device performance. The need of highly sensitive structural probing techniques has increased dramatically with the continuous downscaling the semiconductor devices to improve electrical performance. Due to scaling-related new emerging based problems, new or structurally modified materials will have to be used in crucial parts of the future complimentary metal-oxide semiconductor (CMOS) devices. Synchrotron radiation based spectroscopies can provide the crucial information to correlate the local structural modifications introduced by to new materials or variations in the synthesis conditions. In this talk, recent examples of synthesis conditions versus structure variations as probed by x-ray absorption spectroscopy in thin films of CMOS devices will be presented. Selected examples will be on 1-) Hf based ferroelectric devices and high-k materials 2-) The identification of the stabilized crystal phases in the nickel silicide formation process is crucial, as it was shown that a Si rich Ni silicide layer at the NiSi<sub>2</sub>/Si interface causes a significant reduction in the electron Schottky barrier height (SBH). 3-) Nb-based Nb<sub>2</sub>O<sub>5</sub>-PbO-GeO<sub>2</sub> (NPG), glass photonic thin films where interesting optical characteristics such as observed high nonlinear third order optical susceptibility due to subtle structural variations in Nb local environment 4-) Clustering of the dopant (arsenic) in ultra shallow junctions in source and drain regions leading to electrical deactivation. Quantitative x-ray absorption spectroscopy analyses in these structures based on the data acquired at the National Synchrotron Light Source (NSLS and NSLS -II) of Brookhaven National Laboratory will be presented.

**Keywords:** Synchrotron Based Spectroscopy

**INVITED SPEAKER**

**Id-715**

**Current Advances and Challenges of Label-Free SERS Application in Bacterial Infection and Antibiotic Resistance**

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**Abstract:** Infectious diseases caused by bacterial pathogens are critical public issues. In addition, due to the overuse of antibiotics, many multidrug-resistant bacterial pathogens have been widely encountered in clinical settings. Thus, the fast identification of bacteria pathogens and profiling of antibiotic resistance could greatly facilitate the precise treatment strategy of infectious diseases. So far, many conventional and molecular methods, both manual or automatized, have been developed for in vitro diagnostics, which have been proven to be accurate, reliable, and time efficient. Although Raman spectroscopy (RS) is an established technique in various fields such as geochemistry and material science, it is still considered an emerging tool in researching and diagnosing infectious diseases. Based on current studies, it is too early to claim that RS may provide practical guidelines for microbiologists and clinicians because there is still a gap between basic research and clinical implementation. However, due to the promising prospects of label-free detection and noninvasive identification of bacterial infections and antibiotic resistance in several single steps, it is necessary to have an overview of the technique in terms of its strong points and shortcomings. Thus, in this study, we went through recent works of RS in the field of infectious diseases, highlighting the application potentials of the technique and current challenges that prevent its real-world applications.

**Keywords:** Raman spectroscopy; Bacterial pathogen; Machine learning; Infectious disease; Antibiotic resistance

**INVITED SPEAKER**

**Id-720**

**Raman Spectroscopy Applied on Living Samples: Monitoring of Algal Cells  
Production in Photobioreactors**

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**Abstract:** Raman spectroscopy offers a promising technique for rapid and non-destructive analysis in several domains. The main objective is simplifying the analysis process and reducing the investigation time of samples. The high demand on microalgae-based products promotes its bioproduction on a large scale resulting in a need to optimize the bioprocess monitoring and the development of new analytical tools. The main approaches showing the use of Raman spectroscopy for the control of algal bioproduction will be presented in this study. Some algal strains were produced under different conditions to evaluate the ability of this technique to monitor the physiology of cells in their complex culture environment. The obtained Raman spectra reflect the molecular composition of the biological samples without any extensive preparation or the use of chemical reagents. The statistical exploration of the data shows good classification efficiency for each physiological growth phases of algal cells. Regardless of the advantages offered by this technique, many challenges remain for its application in real conditions. The automation of the approach is currently one of our priorities to scale up the technology. The first tests done, with our developed system, in an industrial algal platform prove the ability of the automated system to monitor the algal production in field conditions. However, the main challenges will be the automation of the whole approach, including the chemometric models, to simplify its use by an unqualified user. Reducing the prices of spectrometers is also very important to help this technology to become widely used and transferred to many other bioprocess domains.

**Keywords:** Microalgae; Monitoring; Bioprocesses, Raman spectroscopy; Chemometrics



**INVITED SPEAKER**

**Id-723**

**Clarifying Structure of Aqueous Solutions by Computationally Supported Spectral Analysis**

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**Abstract:** Water is a unique condensed-state medium that plays a vital role in all aspects of life. In particular, the structures and properties of biomolecules are dependent on their interaction with surrounding water, which also strongly affects their vibrational and electronic spectra. This makes the spectra a valuable source of information on aqueous biomolecules and, at the same time, extremely complicates the spectra interpretation. To alleviate this task, input is required from quantum chemical calculations at computational levels that match the experimental resolution and accuracy. We will discuss computational studies of the UV-Vis. and Raman spectra of aqueous nucleobases and some antiviral drugs in biologically relevant environment. The cluster modeling will be shown to deliver valuable information on the structure of hydration shell of these molecules, their inter- and intramolecular hydrogen bonding, and impact of water on geometry of the dissolved species, in particular – on their tautomeric and conformational equilibria. Possible applications of the developed technique in spectroscopic analysis of other liquids will be discussed.

**Keywords:** UV-Vis and Raman spectra; quantum chemistry; tautomers; conformers; hydrogen bonding

INVITED SPEAKER

Id-727

**Development of Functionalized Carbon Nanotubes and Graphene Composites to Inhibit Single- and Multi-Species Biofilms in Medical Devices**

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**Abstract:** The insertion or implantation of medical devices into the human body has become a recurrent strategy to replace or even repair damaged organs. However, their use is related to a high incidence of device-associated infections, which are mainly caused by bacterial adhesion and biofilm formation on their surfaces, and may represent 50 to 70% of healthcare-related infections. The potential use of carbon materials such as graphene and carbon nanotubes (CNTs) has been investigated to produce coatings for medical devices. In this work, two case studies are presented where nitric acid-functionalized CNTs (NA-CNT) or nitrogen-functionalized graphene nanoplatelets (N-GNP) have been incorporated into a polydimethylsiloxane (PDMS) matrix. The antibiofilm activity of NA-CNT/PDMS composites was assessed against *Escherichia coli* and *Staphylococcus aureus* after 24 h of biofilm formation. Reductions between 30 and 45% in the number of culturable cells were obtained for single-species biofilms depending on the thermal treatment applied to NA-CNT. It was shown that this functionalized carbon material changes the membrane permeability of both Gram-negative and Gram-positive bacteria, while it only induces the production of reactive oxidative species (ROS) in Gram-positive bacteria. Furthermore, NA-CNT composites did not impact HK-2 cell viability, confirming their biocompatibility. The performance of the synthesized N-GNP/PDMS composites was tested against single- and multi-species biofilms of *S. aureus*, *Pseudomonas aeruginosa*, and *Klebsiella pneumoniae*, the most common pathogens associated with urinary tract infections. Biofilms were formed for 24 h in an artificial urine medium. In single-species biofilms, the N-GNP/PDMS composites were able to reduce biofilm culturability by up to 50%. In turn, multi-species biofilms seemed to be less susceptible to the activity of the composites, suffering only a 40% reduction in the total number of biofilm cells, as confirmed by confocal microscopy analysis. In Gram-negative bacteria, N-GNP increases cell metabolism as a response to oxidative stress, whereas in Gram-positive bacteria, this carbon material causes loss of membrane integrity, induces changes in cell metabolism and triggers ROS

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production. Overall, the synthesized composites reduced bacterial biofilm formation, demonstrating the potential of functionalized carbon materials as coatings for medical devices.

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INVITED SPEAKER

Id-727

**Examination of Phase Transformations in Single Metal and Alloy Nanoparticles by in Situ Valence Electron Energy Loss Spectroscopy**

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**Abstract:** A fundamental understanding of the physical and chemical properties of nanosized materials remains among the grand scientific challenges of materials science and nanotechnology. In this work, we tackle the problem by experimental study of phase transformations, structure and morphology in nanosized metal and binary alloy nanoparticles using advanced TEM techniques.

An aberration-corrected scanning transmission electron microscope (STEM) has emerged as a powerful tool for the imaging of nanomaterials with atomic spatial resolution. *In-situ* STEM allows real-time characterization of nanomaterials behaviour under various external stimuli. Here, we explore the power of electron energy loss (EEL) spectral imaging (SI) in STEM for mapping phase states and composition in single nanoparticles at different temperatures. In the first part of the talk, results of studies of melting of single Sn and Sn-Ge nanoparticles using high-resolution HAADF-STEM imaging and valence EELS mapping will be presented. We revealed the surface pre-melting effect and assessed the density of the surface overlayer on a single Sn nanoparticle. Few-monolayer-thick disordered phase nucleated at the surface of the Sn particle at a temperature  $\approx 25\text{K}$  below the melting point and grew into the solid core (up to a thickness of  $\approx 4.5\text{ nm}$ ) with increasing temperature until the whole particle became liquid. We found that the disordered overlayer was not liquid but a quasi-liquid one with a density intermediate between that of solid and liquid Sn. The formation, morphology, and temperature stability of phases in a limited volume of Sn-Ge Janus nanoparticles will be discussed in the second part of the talk. The composition of the liquid phase was determined in a temperature range of  $232\text{-}750^\circ\text{C}$  using EDX and valence EELS techniques and the phase diagram for a single Sn-Ge nanoparticle was assessed. The efficiency of plasmon peak energy mapping for the investigation of interface interactions in two-component nanoparticles will be shown.

**Keywords:** Nanoparticles, Electron Energy Loss Spectroscopy, Alloy

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INVITED SPEAKER

Id-731

**Preparation and Oxidation Resistance of Silicide Coating on Tungsten Substrate**

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**Abstract:** As a very important high-temperature structural material, tungsten has many attractive advantages, such as high melting point, high strength and excellent abrasion resistance, thermal shock resistance and corrosion resistance. However, the poor high-temperature oxidation resistance of tungsten limits its application in high-temperature, high-load, and high-oxidation environment. Surface coating technology is an effective way to balance high-temperature mechanical property and high-temperature oxidation resistance of materials. Pack cementation technique was adopted to prepare the silicide coatings on pure tungsten this work. Both the microstructural characteristics of the coatings before and after high-temperature oxidation were analyzed by means of scanning electron microscopy (SEM), energy dispersive spectrometer (EDS) and X-ray diffractometer (XRD). The oxidation resistance of the coatings was revealed clearly. The silicide coating and Y modified silicide coating are prepared on the pure tungsten by pack cementation. The thickness, microstructure and oxidation resistance of the silicide coating prepared by adding and without adding  $Y_2O_3$  are compared. After the pack cementation at 1250 °C/4 h, the thickness of the coatings can reach about 110 $\mu$ m. Both coatings have a two-layer structure, the outer layer (main layer) is  $WSi_2$ , the inner layer (transition layer) is  $W_5Si_3$ . There are discontinuous columnar structure regions (two-phase zone) between the outer layer and the inner layer. Both coatings are uniform and compact, which are well bonded with the substrate. The Y modified silicide coating shows better oxidation resistance. After oxidation at 1350 °C for 10h, the oxide film is compact and complete, and the coating has no obvious defects. The main phase of the oxide film is  $SiO_2$ , which can protect the matrix from oxidation at 1350 °C/10 h. Therefore, by improving the adhesion of the oxide film, Y element can enhance the anti-spalling ability of the oxide film and improve the high-temperature oxidation resistance of the matrix. The temperature and time of pack cementation can affect the microstructure, composition distribution and defect formation of the coatings. The thickness of the coating increases with increase in the pack cementation temperature and time. The structure of the coating changes when prepared at a higher temperature (1350 °C) and a longer time (6 h). The degenerate layer  $W_5Si_3$  appears above the main layer  $WSi_2$ , and there are obvious cracks and hole defects. Therefore, considering the thickness and quality of the coatings, the optimum pack cementation process parameter of the coatings are determined to be 1250 °C/4 h. At 1250 °C, the growth kinetics of silicide coating and Y modified silicide coating both conform to parabolic laws, and the parabolic rate constant of Y modified silicide coating ( $3.67 \times 10^3 \mu m^2/h$ ) is smaller than that of silicide coating ( $4.25 \times 10^3 \mu m^2/h$ ).

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**Keywords:** Tungsten; Pack cementation; Silicide coating; Oxidation resistance; Microstructural analysis.

INVITED SPEAKER

Id-735

**Analyses of Iron Species, Metals, and Pigments in The Iron-Hyperaccumulator  
Moss *Scopelophila Ligulata***

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**Abstract:** Mosses have been used as biomonitors for heavy metal pollution, and some are known to be metal hyperaccumulators. *Scopelophila ligulata* is a Fe-hyperaccumulator moss; however, the mechanism of Fe accumulation remains unknown and the effects of Fe on pigments remain unclear. To understand the mechanism, we determined Fe species in *S. ligulata* samples. The moss samples were collected from four sites in Japan. The concentrations of Fe, P, S, Cl, and K in them were measured by induced coupled plasma mass spectrometry. Fe species in some of them were determined by Mössbauer spectroscopy and were confirmed by X-ray diffraction analysis. Fe species in *S. ligulata* samples were determined to be jarosite, ferritin, high-spin Fe(II) species, and akaganeite. To our knowledge, this is the first report on the biomineralization of jarosite in mosses. This result, combined with the fact that bacteria, a fungus, and a grass mineralize jarosite, suggests that its biomineralization is a common characteristic in a wide variety of living organisms. These findings indicate that the biomineralization of jarosite occurs not only in the region-specific species but in species adapted to a low-pH and metal-contaminated environment in different regions, provide a better understanding of the mechanism of Fe accumulation in the Fe-hyperaccumulator moss *S. ligulata*, and offer new insights into the biomineralization of jarosite. To clarify the effects of Fe on pigments in the *S. ligulata* samples, we measured their metal and pigment concentrations. The Fe concentration was 10–61 times higher than that in normal mosses, confirming that the moss is a Fe-hyperaccumulator. Two black samples of *S. ligulata* had the first and second highest Fe concentration (2.9 and 2.2 wt%), which explains their color and indicates that the excess amount of Fe is distributed through the plant body. Moreover, we observed that the concentration of Ca is negatively correlated with the concentrations of pigments and, conversely, that the concentration of K is positively correlated with the concentrations of pigments. This inverse relationship between Ca and K can be explained by the reduced uptake of K in *S. ligulata* in response to Ca stress, which is supported by the fact that the concentration of Ca is negatively correlated with that of K. These findings provide a better understanding of the relationships between metals and pigments in the Fe-hyperaccumulator moss *S. ligulata*.

**Keywords:** Metal-Hyperaccumulator, Moss, Iron, Pigment, Mössbauer Spectroscopy

INVITED SPEAKER

Id-737

**Carbon Nanomaterials with Performance in EMI Shielding: Growth, Structuring and Characterization of Materials**

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**Abstract.** Carbon nanomaterials (CNs) have been widely used in various fields such as electronic devices, sensors, and batteries due to their unique mechanical, thermal, and electrical properties. One of the primary challenges is to control the size, shape, and reproducibility during synthesis. Additionally, the properties of the CNs can be significantly influenced by the synthesis conditions such as temperature, pressure, and reaction time. The aim of this study is to examine the characteristics of different CNs synthesized using plasma enhanced chemical vapor deposition (PECVD) on large surfaces and different substrates by Raman spectroscopy and Raman mapping. These CNs include carbon nanotubes (CNTs), mono/multilayer graphene, vertical graphene (GNW), carbon nano-onions (CNO), and nanocrystalline graphene (NCG). Raman spectrometry is used to investigate the intensity ratio of the D to 2D band in Raman scattering, to assess the material type and defect density of CNs. These analyses explain the atomic vibrational properties of carbon specific for each type of material and provide an indicator of the quality of the nanomaterial required to optimize its performance for applications. Raman mapping was successfully applied to characterize the structural changes of CNs with a large surface area. The results showed us that Raman spectroscopy and mapping represent a powerful combination for the in-depth analysis of the characterization of these types of materials. In addition, the current challenges in the synthesis and application of these CNs are highlighted for each type of nanomaterial depending on its properties. In the context of electromagnetic interference (EMI) shielding, the unique properties of these CNs make them promising candidates for mitigating EMI effects. The structural composition and defect density revealed through Raman spectroscopy play a crucial role in influencing the electromagnetic properties of these nanomaterials. Carbon nanotubes and graphene, in particular, exhibit exceptional electrical conductivity and mechanical strength, making them effective in absorbing and dissipating electromagnetic radiation. The ability to precisely control the synthesis conditions further allows tailoring the electromagnetic properties of CNs to enhance their efficiency in EMI shielding applications. The findings from this study contribute valuable insights into the potential of CNs for addressing EMI challenges, paving the way for the development of advanced materials with superior electromagnetic interference shielding capabilities.



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**Keywords:** Carbon nanomaterials; Raman spectroscopy; Nanomaterial characterization; Electromagnetic interference shielding

**Acknowledgment:** This work was supported by grants of the MRID, CNCS-UNEFISCDI, PN-III-P2-2.1-PED-2021-4158 and MicroNEx, Contract no PFE541, MICRO-NANO-SIS PLUS Program, project 19160102; PNCDI IV (2022-2027) core project number 2307, 23/PNRR-III-C9-2022-I8 PNRR/2022/Component 9/Investment 8 Contract 760101/23.05.2023.

**INVITED SPEAKER**

**Id-747**

**Quantitative Interpretation of Nanoparticle X-ray Photoelectron Intensities**

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**Abstract:** Determining shell thicknesses and chemistry of Core-Shell Nanoparticles (CSNPs) presently constitutes one of the most important challenges related to characterisation of nanoparticles. While for particle number concentration various routine analysis techniques as well as methods providing reference measurements have been or are in the process of being developed, one of the most promising candidates for shell thickness determination is x-ray photoelectron spectroscopy (XPS). Different approaches to quantify shell thicknesses will be presented and compared. These comprise: (1) The in- finitesimal columns model (IC), (2) Shard's empirical formula (TNP-model) and (3) SESSA (Simulation of Electron Spectra for Surface Analysis) simulations with and (4) without elastic scattering. CSNP XPS intensities simulated with SESSA for different combinations of core/shell-material combinations for a wide range of core and shell thick- nesses have been evaluated with the TNP-model and the retrieved thicknesses are in good agreement with the nominal thickness, even when elastic scattering is turned on during the simulation, except for pathological cases. For organic shell materials these simulations fully confirm the validity of the (much simpler) TNP-method, which also coincides with the IC model. Experimental data on of a round robin experiment of PMMA@PTFE CSNPs involving three research institutions were analysed with the aforementioned approaches and show a good consistency in that evaluations of the shell thicknesses among the institutions agree within 10% (and are in good agreement with the nominal shell thickness). This consistency is promising since it suggests that the error due to sample preparation can be controlled by following a strict protocol. Within this field, SESSA (Simulation of Electron Spectra for Surface Analysis) is a software that provides a means to simulate peak intensities as well as entire spectral regions for photoelectron spectroscopy. X-ray photoelectron spectra can be simulated for several types of nanostructures, such as CSNPs. SESSA can also be utilized in more complex cases, e.g., if the nondipolar terms in the photoelectric ionization cross section need to be taken into account, a typical situation encountered in spectroscopy using synchrotron radiation. We describe features of the software and present several applications related to analysis of nanoparticles by means of photoelectron spectroscopy.

**Keywords:** X-ray photoelectron, electron, spectroscopy, nanoparticle, core-shell nanoparticle

INVITED SPEAKER

Id-749

**LITES: a Facility for Spectroscopic Remote Sensing and in-situ Atmospheric studies**

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**Abstract:** Atmospheric aerosols such as mineral dust, bio-aerosols and volcanic ash can be transported over tens of thousands of kilometers from its source regions. Despite an abundance of observations and modelling studies, large gaps remain in our understanding of the effect of mineral dust on air quality, human health, and climate. Raman spectroscopy represents a particularly powerful tool for laser remote sensing because it allows us to both identify and quantify the chemical constituents in a complex aerosol mixture - as is often the case for atmospheric aerosol pollution. Nowadays, Raman lidar allows for an independent quantitative measurement of aerosol backscatter and extinction coefficient profiles with the use of Raman scattering from nitrogen or oxygen molecules. Previous works have shown that the detection of Raman scattering by silicone dioxide in a lidar receiver can be used to infer the concentration of mineral dust in the atmosphere. In recent years we have been developing a novel multi-channel spectrometric lidar system. This new approach will be used for detecting characteristic features of Raman spectra, which subsequently can be used for inferring chemical signatures of aerosol particles. To achieve this goal, we need currently unavailable information on the Raman spectra of aerosol species commonly found in the atmosphere. We will present design and experimental results from a lidar facility that has been designed and built at the University of Hertfordshire. LITES (Lidar Innovations for Technologies and Environmental Sciences) allows for testing, developing and measuring a multitude of, e.g. climate-change relevant parameters of atmospheric particulate pollution and photo-chemically reactive trace gases. The core of LITES consists of a lidar spectroscopy instrument. In this contribution we present the design and specifications of the facility, its performance and potential applications. We will show examples of measurements of range-resolved pure rotational Raman spectra and rotational-vibrational Raman spectra of air molecules, aerosol and gas pollution. In this contribution we will present also experimental results of Raman and fluorescence spectra of a collection of 30 different aerosol samples. These samples are well characterized in terms of their chemical composition. The samples include, mineral dust (quartz, hematite, kaolinite, barite, calcite etc.), and bio-aerosols. We investigated these samples under laboratory conditions with a Raman microscope. The setup includes an Olympus BX51TRF-6 microscope with objective-lens magnifications x5, x10, x20, x50, and x100. The setup allow for a spatial resolution better than 1  $\mu\text{m}$ . The Raman and fluorescence spectra are obtained with a HORIBA 1250M Research Spectrometer that uses four different gratings. The spectral

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resolution thus is better than  $1\text{cm}^{-1}$ . Data acquisition is done by a PI-MAX4 ICCD camera, an ANDOR iXon 3 EMCCD camera, photo multiplier tubes, and Si and InGaAs detectors.

INVITED SPEAKER

Id-750

Characterization of Composite Materials

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**Abstract.** Composite materials based on different polymers and fillers (nano- or micro-scale) are a widespread topic in academic and industrial research. Composites are multifunctional innovative materials or multicomponent systems in which the dispersion of the fillers and the interactions between the components also have an effect on the surface, mechanical, thermal, physicochemical, antimicrobial and other properties of the composites. Widely used polymers such as poly(vinylidene fluoride) (PVDF) and its copolymers (e.g. PVDF-HFP) are used in various fields. The polycrystalline nature of PVDF polymers strongly depends on the preparation method and the type of fillers, which influence the presence of polar and non-polar phases. The presence of polar phases has been studied in detail due to their electroactive properties. PVDF-based composites are therefore used in numerous applications such as batteries, membranes, sensor systems, dielectric devices, nanogenerators, water purification systems, smart scaffolds and other biomedical devices due to their good mechanical strength, chemical inertness, thermal stability and excellent biocompatibility. The Federal Drug Administration (FDA) permits the use of PVDF in the food, biochemical and pharmaceutical industries. Therefore, the antimicrobial and antifouling properties of PVDF-HFP-based composites were investigated on PVDF-HFP/PVP, PVDF-HFP/PEO/MoO<sub>3</sub>, PVDF-HFP/PVP/MoO<sub>3</sub> nanocomposites. The development of antimicrobial and antifouling surfaces plays an important role in preventing the transmission of microbial infections and on the survival time of microbes on surfaces. The use of these surface coatings in high-touch locations can reduce the incidence of infectious diseases in various environments (food contamination, door handles, hospital beds and documentation, shopping centers). However, these special properties of PVDF-based polymer composites also offer many opportunities for microscopic and spectroscopic characterization at the micro- and nanoscale. Optical microscopy, scanning electron microscopy (SEM) and atomic force microscopy (AFM) are presented as characterization methods for the surface properties. The topography, the surface roughness, and the micro-/nano-structuring of the surface have a significant influence on the interaction of microbes with the surface and thus on the ability to form biofilms. In addition, spectroscopic methods (Raman spectroscopy, Fourier transform infrared spectroscopy - FTIR, UV-Vis spectroscopy, dielectric spectroscopy) are used to monitor the interactions between the components and the substrate, which have an impact on the improvement of the properties compared to the pure polymer blend. The results of all these spectroscopic and microscopic analyses on PVDF-HFP based polymer nanocomposites are presented.

**Keywords:** polymer nanocomposites; spectroscopy; microscopy; PVDF-HFP; antimicrobial.

**INVITED SPEAKER**

**Id-755**

**Bioactive Glasses/Glass-Ceramics/Metal Nanoparticles Based Composites for  
Tissue Engineering Applications**

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**Abstract.** A superior scaffold must be crafted to mimic the innate regenerative processes of the human body. To achieve this, the scaffold must meet several key criteria: exceptional bioactivity, strong biocompatibility, osteoconductivity, osteoinductivity, promotion of angiogenesis, appropriate structural and mechanical characteristics, and biodegradability. Particularly, alginate (Alg) and pullulan (Pll) were widely used as biomaterials for bone tissue engineering. At the same time, bioactive glasses and glass-ceramics (GC) with gold nanoparticles (AuNPs) were found to stimulate keratinocyte cell proliferation. On the other hand, the use of CuO is justified by the improvement of the cell viability and angiogenesis properties as well as a good antibacterial effect. Taking into consideration the above-mentioned aspects, our research group developed and investigated a series of novel composites based on a bioactive matrix (i.e., silicate glasses or GC), and biopolymers like Alg, Pll) containing CuO or differently shaped AuNPs by assessing their bioactive, biocompatible, and antibacterial properties. Our first interest was to combine Cu-containing bioactive GC-based composites with Alg and Pll natural polymers for the synthesis of new biocompatible hydrogels and their use as support for in vivo tissue regeneration with antibacterial properties. It was shown that bioactive GC with relatively small amounts of CuO (i.e., 0.5 and 1.5 mol%) have excellent cell viability and good antibacterial effect against *Staphylococcus aureus*. Further, evaluating the bone regeneration response of these Alg-Pll-GC composite scaffolds in an experimental long bone defect orthotopically implant it proved a very good in vivo quality. Other studies demonstrated that Alg-Pll-bioactive glasses with AuNPs (Alg-Pll-BGAuSP) are promising materials for soft and bone engineering endeavors. The composites, including the control sample, were implanted in bone defect in Wistar rats for 8 weeks, after that the remained materials were recovered. Based on the in vivo subcutaneous analyses the polymer composites with BGAuNP have shown excellent biocompatibility, exhibiting marked angiogenesis. At the same time, tissue proliferation was confirmed by a high number of Vimentin-positive cells. The obtained results indicated that these composites can be real promising candidates for use in future tissue engineering applications.

**Keywords:** tissue engineering, composites, bioactive glass-ceramics, biopolymer, metal nanoparticles

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**INVITED SPEAKER**

**Id-756**

**Vibrational Spectroscopic Investigations on Pharmaceuticals**

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**Abstract.** Nowadays, medicine focuses on the individual diagnosis and treatment of patients. Although this path is still in its beginning, every small step in this direction will be a big one towards achieving this goal. To understand the behavior of a molecule in different interactions in various environments, a full analysis of its chemical and physical properties is required. Vibrational spectroscopic methods (Raman and FT-IR) combined with density functional theory (DFT) calculations are perfect tools for this aim. But, sometimes, weak Raman signal intensity and fluorescence interference make the use of Raman spectroscopy impossible. Surface-enhanced Raman spectroscopy (SERS) can overcome these drawbacks; it allows the detection of molecules at very low concentrations due to the enhancement of the Raman signal of species adsorbed on a metal surface. SERS spectroscopy is also used to understand the action of drugs as it is essential to identify any alteration of the adsorbed species structure relative to that of the free molecule. In these trials, the metal surface can serve as a mimic of a biological interface and, after clarifying the adsorption mechanism of a molecule on this surface, the study can be extended to adsorption on membranes or other biological surfaces of interest for therapeutic treatments to imitate the adsorption of drugs into the organism. Additionally, due to its ability to detect analytes at low concentrations, SERS is a suitable technique in therapeutic drug monitoring, which could help physicians use the optimal dose to achieve a more effective treatment tailored to each patient. Taking into consideration these aspects we carried out in our group detailed vibrational (FT-IR and Raman spectroscopy) investigations coupled with DFT calculations on different pharmaceuticals such as anti-inflammatory drugs, antibiotics, tranquilizers and sedatives, chemotherapeutics, etc. to provide insights into their structure. Furthermore, by analyzing the SERS spectra, the adsorption behavior i.e. chemisorption or physisorption, the adsorption site, the orientation of the adsorbed molecules on the metal surface, was elucidated. Regardless of its established sensitivity, the use of SERS in quantitative analysis is still a challenge. To make the step towards clinical applications, identical results need to be obtained regardless of location, equipment, or user, and interlaboratory studies are currently the best way to achieve this. A recent study aimed to assess the reproducibility and trueness of a quantitative SERS method and to compare different methods suggested that SERS is a method that can be used by different laboratories if it is very well-defined. The tested methods produced a range of reproducibility results, but the best ones were reasonably reproducible, with an average standard error of performance as low as 12% and 13%. The obtained results were encouraging since

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different instruments were used over a long period, with different setup and acquisition parameters. The next step should be the evaluation of each source of experimental uncertainty (e.g., substrates, instruments) for the best performing methods. Nevertheless, it is obvious that Raman and SERS are promising tools for medical applications such as therapeutic drug monitoring or personalized medicine.

**Keywords:** FT-IR and Raman spectroscopy, DFT calculations, SERS, pharmaceuticals, adsorption



**INVITED SPEAKER**

**Id-758**

**Going to Extremely Low Doses: Electron Crystallography with The Dose-Symmetric Electron Diffraction Tomography**

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**Abstract:** The understanding of the properties of materials closely relies on the knowledge of their crystallographic structures. It is therefore paramount to dispose of suitable methods and instruments in order to determine these structures if we want to develop new and better materials. For materials that can be grown to stable single crystals of at least a few tens of micrometers in diameter the crystallographic gold standard is single crystal X-ray diffraction (SCXRD). However, there is a wealth of materials that exist only in nanometric crystals, because the growth of bigger crystals is either impossible or so complicated that it is not reasonable to spend enough time and resources to grow bigger crystals before knowing their potential for research or applications. In these cases, SCXRD is no longer an option and new characterization methods need to be optimized. Among these nanometric crystals, radiation sensitive materials are the most difficult materials to study. The challenge here is to get a maximum of information out of these particles before the radiation damages them to a point where their structure is altered. Both characteristics, the small size and the beam sensitivity, call for electron diffraction as a privileged investigation tool. The strong interaction of electrons (as compared to X-rays) with matter allows single crystal diffraction experiments on nanometer-sized crystals and for the same amount of beam damage, electron diffraction yields more information than X-rays. For this reason, different 3-dimensional electron diffraction (3D ED) techniques like the low-dose electron diffraction tomography (LD-EDT) [1] have been developed in recent years that use only low electron doses. Nevertheless, in some cases even these low doses can cause structural damage in the crystals. In order to further lower the necessary dose to obtain complete data sets without damaging the crystals, we developed the dose symmetric electron diffraction tomography (DS-EDT) method [2], combining the low-dose electron diffraction tomography (LD-EDT) technique with the dose-symmetric tomography scheme known from cryo-EM. In order to reduce the dose on an individual crystal and still obtain enough data for a structure solution and refinement, we partition the dose over several crystals. The individual datasets are then merged in order to achieve the necessary completeness. On two test structures we first show that merging of data from small domains of the reciprocal space is indeed sufficient to obtain reliable data for structure solution and refinement. Second, we show on the beam sensitive manganese formate that high-quality data can be obtained on a few frames while the frames that have suffered from beam damage can still be used to determine the orientation matrix and the unit cell of the crystals. The results from the dynamical refinement on the obtained data show a high accuracy of the atom positions. In

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this way, DS-EDT can reduce the total dose on an individual crystal by an order of magnitude with respect to the already very dose-efficient LD-EDT.

**Keywords:** Electron Crystallography; 3D-ED; Beam Sensitive Materials; Low-Dose Technique, Structure Solution; Structure Refinement

**INVITED SPEAKER**

**Id-761**

**Surface Termination-Driven Optical Behavior in MXene Nanoflakes**

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**Abstract:** Two-dimensional (2D) transition metal carbides, nitrides, and carbonitrides, known as MXenes, represent an expanding category of 2D materials. With their diverse compositions and various surface terminations, they hold promise for advancing the development of innovative devices. In this study, employing quantum-mechanical simulations via time-dependent density functional theory, we examine the influence of the M element (Ti or V) and surface terminations (T<sub>x</sub>, such as F and O) on the optical and plasmonic properties of M<sub>2</sub>CT<sub>x</sub> MXene nanoflakes. Our investigation unveils the emergence of localized surface plasmon resonances (LSPRs) in MXene nanoflakes. Intriguingly, the Janus MXene nanoflake Ti<sub>2</sub>CFO (with F termination on the top surface and O termination on the bottom surface) exhibits the most intense and narrowest infrared LSPR, attributed to its largest out-of-plane time-dependent dipole moment. These findings offer insights valuable for researchers exploring MXene plasmonics.

**Keywords:** DFT, TD-DFT, Plasmons

INVITED SPEAKER

Id-764

**Understanding Organic Crystal Surfaces Using Polarized Raman Spectroscopy**

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**Abstract.** Physicochemical properties including agglomeration and aggregation impact pharmaceutical materials in both the final drug form and downstream manufacturing processes. These behaviours are governed by the interactions at the surfaces which in turn depend on both the identity and orientation of exposed functional groups, meaning an in depth study on these surfaces is crucial in predicting and controlling the properties of pharmaceutical materials. Powder X-ray diffraction and Angle Resolved Polarised Raman Spectroscopic (ARPRS), in combination with computational modelling of the data, offers a method of identifying crystal facets for samples too large for standard single-crystal X-ray diffraction face indexing. By taking Raman spectra at different sample orientation angles and monitoring the change in normalised intensity for each vibrational mode, understanding of the orientation of functional groups can be gained. This study also demonstrates that while single Bragg peaks observed due to preferred orientations in powder X-ray diffraction patterns of crystal facets are useful for facet assignment, subtle variations in crystal structure can be reflected in peak position. These shifted peaks can suggest assignments not observed upon inspection of the particle morphology however the ARPRS data helps to reveal more consistent facet assignments. This work also explores differences in polarisation symmetry between vibrational bands, in addition to facet identification, that arise because of changes in vibrational mode net stretching direction. This technique will be applied to study model drugs such as paracetamol, aspirin and metacetamol.

**Keywords:** ARPRS; surfaces; pharmaceuticals; PXRD; DFT.

**Acknowledgment:** This talk will be dedicated to my late mentor Prof Patrick McArdle. I would like to thank the Royal Society for my Olga Kennard Fellowship and acknowledge Astra Zeneca and the EPSRC ICASE funding for Dave's studentship.

ORAL PRESENTATION

Id-724

**Preparation of Ionic Liquid Electrolyte Suitable for Low Temperature Environment and Its Lithium Ion Battery**

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**Abstract.** Lithium ion battery, as an important energy storage device, has a long cycle life, large energy and power density, and is widely used in various electrical equipment. As an important part of lithium ion battery, electrolyte plays an important role in battery performance. At present, as the main commercial electrolyte, organic liquid electrolyte has the advantages of high ionic conductivity and good interfacial wettability. However, due to the flammable and volatile characteristics of organic liquid electrolyte, it will lead to combustion and explosion accidents. In addition, at low temperature, the migration number of lithium ions in the electrolyte decreases, and the impedance of the electrolyte electrode interface increases, which makes the reaction kinetics of the battery slow and makes the capacity decay rapidly. Therefore, the application at low temperature is still limited. Ionic liquid is a kind of room temperature molten salt with stable chemical properties, which has excellent solubility and high conductivity. Its application in electrolytes has become a recent research hotspot. Because of the large volume of the constituent ions, ionic liquids cannot form a stable lattice, so they can maintain the state of liquids at room temperature, with a wide range of liquid temperatures. Benefiting from the structural adjustability of ionic liquids, the conductivity, viscosity and melting point of ionic liquids can be improved by changing the structure and composition of anions and cations to meet the application requirements of batteries in low temperature environments. Ionic liquids 1-butyl-3-methylimidazolium bis (trifluoromethyl) sulfonimide ([BMIM]TFSI) with good electrochemical stability and 1-ethyl-3-methylimidazolium tetrafluoroboric acid ([EMIM]BF<sub>4</sub>) with high conductivity were prepared by ion exchange method, and their physicochemical and electrochemical properties were characterized. The effect of different ratios on its electrochemical performance was studied, where x was 0.2, 0.4, 0.6, 0.8, respectively. The results show that when x=0.2, the comprehensive performance of (1-x)[BMIM]TFSI-(x)[EMIM]BF<sub>4</sub> is the best. The viscosity and conductivity at 20°C are 48.0 mPa·s and 6.25 mS·cm<sup>-1</sup>, respectively. In addition, the electrochemical stability window (5.4V) and lithium ion migration number (0.4) of electrolyte (1-x)[BMIM]TFSI-(x)[EMIM] BF<sub>4</sub>-10%Li at this ratio are higher than those of only [BMIM]TFSI-10%Li or [EMIM]BF<sub>4</sub> -10%Li. when x is 0.2, the specific discharge capacity of lithium ion battery Li/(1-x)[BMIM]TFSI-(x)[EMIM]BF<sub>4</sub>-10%Li/LiFePO<sub>4</sub> at 0.1C, 0.2C, 0.5C and 1C is 128.75, 110.1, 68.2 and 24.7 mAh·g<sup>-1</sup> respectively, and the capacity retention rate is 91.7% after the current density returns from 1C to 0.1C. It shows higher charge-discharge specific capacity than only Li/[BMIM]TFSI-10%Li/LiFePO<sub>4</sub>. At 20°C and -20°C, the maximum discharge specific capacity is 134.4 mAh·g<sup>-1</sup> and 114.9 mAh·g<sup>-1</sup> at the charge and discharge rate of 0.1 C, respectively. After 50 cycles, it is reduced to 108.7 mAh·g<sup>-1</sup> and 72.1 mAh·g<sup>-1</sup>

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respectively, and the capacity retention rate is 95.1% and 75.1% respectively. It shows a certain stability of cycle performance, and potential application at low temperature. A series of research results have provided an important basis for the research and development of low-temperature electrolyte and have good application value.

**Keywords:** Ionic liquid, low temperature lithium ion battery, electrolyte, electrochemical performance

ORAL PRESENTATION

Id-757

**Nanoscale Investigations of Complex Microbial Interactions with Extraterrestrial and Terrestrial Minerals Using TEM-Based Approach: Implications for Life on Earth and Beyond**

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**Abstract-** Astrobiology is a young and rapidly developing branch of science that strives to address the question of whether life exists, or has existed, elsewhere in the Universe. Current research activities in the field of astrobiology have evolved at the boundaries of biosphere, geosphere, hydrosphere and atmosphere, exploring the interactions between the biological, geological, hydrological, and atmospheric elements in the Universe. Our recent investigations address the astrobiological implication of microbial-mineral interactions, biosignatures as traces of life that can be detected in the physicochemical conditions beyond Earth, and molecular mechanisms of microbial survival beyond Earth. This abstract summarises some of my contributions in the area of Mars-relevant biosignatures, tungsten-microbial interactions as a microbial strategy to withstand harsh environments, and molecular mechanisms of microbial survival beyond Earth. Our recent study on the Noachian Martian breccia composed of ~4.5 Gyr old Mars crustal fragments, delivered a prototype of microbial life experimentally designed on a real Martian material. This life of pure Martian design is a rich source of Mars relevant mineral and metabolic biosignatures, which may pave the way to efficient nano-assessment of the biogenicity of returned Mars samples. Besides this, I will present experiments on microbial exposure outside the International Space Station (ISS) and survival during interplanetary travel investigated using TEM-based approach. Additionally, some of our recent research has indicated that microbial cells form a robust, tungsten-bearing mineralized cell crust (5,6) that may help them withstand harsh environments. An integrative approach of microbiology, wet chemistry and transmission electron microscopy coupled to spectroscopy nanoanalysis, which has been developed during these investigations, contributes to the advanced development of astrobiological research.

**Keywords:** mineral-transforming archaea; microbial-mineral interactions; transmission electron microscopy; astrobiology; terrestrial and extraterrestrial minerals.

POSTER PRESENTATION

Id-739

**How Does The Health-Promoting Apple Phenolic Phloretin Affect The Cell Ultrastructure in Arabidopsis Shoots?**

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**Abstract:** Phloretin is a phenolic compound from the apple that belongs to the group of dihydrochalcones. The genus *Malus* is a uniquely rich source of dihydrochalcones, accounting for about 97% of the total phenolic compounds in apple leaves and 10-20% of the dry weight of the leaf tissue. Due to its typical dihydrochalcone structure, phloretin is a highly reactive molecule that interacts efficiently with many biological macromolecules. Its reactivity leads to remarkable antioxidant and medicinal properties that have been extensively studied in mammals and humans. However, knowledge about the effects of phloretin on plant organisms is rather scarce. The phytotoxicity of phloretin in plants was first documented by our research group when phloretin was recognised as a potent allelochemical of the apple tree with deleterious effects in plant species outside the genus *Malus*. Research on the model plant *Arabidopsis* [*Arabidopsis thaliana* (L.) Heynh] named the disruption of auxin homeostasis in the roots as the main mechanism of the phytotoxic effect of phloretin. The present study complements previous research with new insights into the ultrastructural changes in leaf mesophyll cells that underlie the growth arrest and decay of the aerial parts of *Arabidopsis* seedlings exposed to phloretin. The effects of phloretin are closely linked to the ultrastructural damage in the leaf mesophyll cells and range from mild effects with short-term treatment to severe effects with long-term treatment. Transmission electron microscopy revealed changes in the morphology of the cell wall, changes in thylakoid organisation, swelling and displacement of chloroplasts after short-term treatment. A significant decrease in the number of starch granules and chlorophyll content in the leaves reflected impaired chloroplast function leading to depletion of starch reserves, starvation of cells and recruitment of micro- and macroautophagic processes for self-maintenance leading to programmed cell death after long-term treatment with phloretin. These results confirm that the sites of action of phloretin in plant and animal cells do not coincide, confirming the safety of its potential application as a new bioherbicidal agent for humans and animals.

**Keywords:** bioherbicides, phloretin, autophagy, programmed cell death



**POSTER PRESENTATION**

**Id-748**

**Characterization of Uncoated and Silver Coated Copper Flake Based Polymer Composites**

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**Abstract:** Polymer composites are materials that consist of two or more different materials. Materials such as metals, polymers, ceramics and organics can be combined to improve their physical properties compared to the neat polymer. In polymer composites, the polymer usually serves as the matrix, while the fillers, which must be well distributed in the matrix, act as reinforcement, filler or are used to provide functional property. Due to its light weight and durability polyethylene, one of world's most widely used polymers, is a promising material for the use as a polymer matrix in polymer-based composites. It has been reported that polymer composites with polyethylene can exhibit various functional properties, such as mechanical reinforcement, thermal and electrical conductivity. To produce conductive polymer composites (CPCs), a polymer matrix should be conductive, or the added filler must be a conductor, e.g. a metallic (copper, silver, etc.), a carbon (graphene, carbon fibers, carbon nanotubes, etc.). The most promising metal used as conductive filler is undoubtedly copper (Cu), as it is cheap and abundant. However, it oxidizes at high temperatures and cannot maintain its high conductivity over a long period of time. For the production of conductive polymer composites using Cu flake particles, it is therefore necessary to protect their surface from oxidation. To improve oxidation stability and conductivity, the surface of the Cu particles can be modified with various materials such as silver (Ag), gold (Au), nickel (Ni), etc. Since Ag is the best inorganic conductive element, it is used to modify the surface of Cu particles, forming core-shell Cu@Ag [3] particles that are more conductive and less susceptible to oxidation. Surface modification of Cu particles with Ag increases the conductivity of the composite and can also have a major impact on network formation in the polymer matrix. In this study, we focus on the production of injection-molded conductive composites based on copper (Cu) or silver-coated copper particles (Cu@Ag) depending on the volume fraction of filler added (up to 40 vol%) to the non-conductive polymer matrix (low density polyethylene – LDPE). Polymer composites were characterized in terms of their thermal, electrical, morphological and spectroscopic properties. Complementary analytical techniques enabled determination of the network formation, which is necessary to significantly improve the electrical and mechanical properties of such composites.

**Keywords:** Polymer Composites, Copper Flakes, Silver Coating, Percolation Threshold

## All Submissions &amp; Topics

Topic	Submission
<b>1 - Applications of Micr</b>	713 - 3D Imaging And Spectroscopy Of Complex Biological Systems At The Sub-Cellular, Cellular And Multicellular Levels
	715 - Current Advances And Challenges Of Label-Free SERS Application In Bacterial Infection And Antibiotic Resistance
	720 - Raman Spectroscopy Applied On Living Samples: Monitoring Of Algal Cells Production In Photobioreactors
	739 - How Does The Health-Promoting Apple Phenolic Phloretin Affect The Cell Ultrastructure In Arabidopsis Shoots?
	752 - Confocal Microscopy Imaging Of Drosophila Melanogaster Embryos Exposed To Tumour Treating Alternating Current Electric Fields
<b>2 - Biomedical applicati</b>	727 - Development Of Functionalized Carbon Nanotubes And Graphene Composites To Inhibit Single- And Multi-Species Biofilms In Medical Devices
<b>3 - Botany</b>	735 - Analyses Of Iron Species, Metals, And Pigments In The Iron-Hyperaccumulator Moss Scopelophila Ligulata
	757 - Nanoscale Investigations Of Complex Microbial Interactions With Extraterrestrial And Terrestrial Minerals Using TEM-Based Approach: Implications For Life On Earth And Beyond
<b>4 - Applications of Micr</b>	723 - Clarifying Structure Of Aqueous Solutions By Computationally Supported Spectral Analysis
	728 - Examination Of Phase Transformations In Single Metal And Alloy Nanoparticles By In Situ Valence Electron Energy Loss Spectroscopy
	750 - Caraceterization Of Composite Materials
	756 - Vibrational Spectroscopic Investigations On Pharmaceuticals
<b>5 - Biomaterials</b>	755 - Bioactive Glasses/Glass-Ceramics/Metal Nanoparticles Based Composites For Tissue Engineering Applications
<b>6 - Composites</b>	733 - Grain Refinement In Snagcu-(Tio2/Zro2/Cuo) Composite Solder Joints
	748 - Characterization Of Uncoated And Silver Coated Coper Flake Based Polymer Composites
<b>7 - Materials for energy</b>	724 - Preparation Of Ionic Liquid Electrolyte Suitable For Low Temperature Environment And Its Lithium Ion Battery
	761 - Surface Termination-Driven Optical Behavior In Mxene Nanoflakes

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<b>8 - Metals</b>	731 - Preparation And Oxidation Resistance Of Silicide Coating On Tungsten Substrate
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<b>10 - Image simulation and</b>	759 - Interconnection Of Microscopy And Radiology In Medical Imaging
<b>11 - Transmission electro</b>	734 - Seeing Matter From Ultra-Small To Ultra-Fast And To Ultra-Cold With Electrons
<b>12 - Advances in Instrume</b>	762 - Structure-Function Correlation In Advanced Materials Using Synchrotron Based Spectroscopy
<b>13 - Raman spectroscopy</b>	716 - Probing The Intermolecular Vibrations And Reorientation In Liquids And Solutions By Femtosecond Raman-Induced Kerr Effect Spectroscopy
	737 - Carbon Nanomaterials With Performance In Emi Shielding: Growth, Structuring And Characterization Of Materials
	749 - LITES: A Facility For Spectroscopic Remote Sensing And In-Situ Atmospheric Studies
	764 - Understanding Organic Crystal Surfaces Using Polarized Raman Spectroscopy
<b>14 - X-ray photoelectron</b>	747 - Quantitative Interpretation Of Nanoparticle X-Ray Photoelectron Intensities