FIRST NORDIC SUB-MICRON IR MICROSCOPY CONFERENCE

15-17 Oct 2025 - Lund, Sweden

PROGRAM & ABSTRACT BOOKLET

Conference Organizers:
Milda Pucetaite
Karina Thånell
Nikolay Vinogradov
Calley Eads
Agnes Paulus
Antti Kalanti

LINXS

PROGRAM

Day 1 **Wed (2025-10-15)**

10:45 – 11:45 – Registration and mingling

11:45 – 12:45 – Lunch

12:45 – 13:00 – Welcome and introduction

Plenary lecture

13:00 – 14:00 – **Dr. Jeremie Mathurin (for Prof. Alexandre Dazzi), University of Paris-Saclay, France**

Introduction and overview of AFM-IR spectroscopy

14:00 – 14:30 – **Dr. Khaled Kaja (for Hartmut Stadler), Buker Corporation, Germany**

AFM-IR spectroscopy instrumentation and possibilities

14:30 – 15:00 – Coffee break

Plenary lecture

15:00 – 16:00 – **Prof. Ji-Xin Cheng, Boston University, USA (online)**

Optical Photothermal Infrared Microscopy: Innovations & Applications

16:00 – 16:30 – **Dr. Miriam Unger, Photothermal Spectroscopy Corporation, Germany**

mIRage for O-PTIR spectroscopy and application possibilities

16:30 – 17:30 - Moderated Q&A to the speakers

Day 2 **Thu (2025-10-16)**

9:00 -10:30 – **Session I:** applications of sub-micron IR spectroscopy

Invited lecture

9:00 – 9:30 – **Dr. Tue Hassenkam, Copenhagen University, Denmark**

NanoIR of biosignatures

9:30 – 9:50 – **Dr. Szymon Tott, NCSR Solaris, Jagiellonian University, Poland**

Deep-dive into cell composition with O-PTIR in water environment

9:50 – 10:10 – **Dr. Crislaine Bertoldi, Lund University, Sweden**

Transforming microplastic analysis: the power of O-PTIR spectroscopy

10:10 – 10:30 – **Dr. Maria Eleonora Temperini, Helmholtz-Zentrum Berlin für Materialien und Energie, Germany**

Multiscale IR Spectroscopy of Proteins at IRIS Beamline

10:30 – 11:00 – Coffee break

11:00 – 12:30 – **Session II:** applications of sub-micron IR spectroscopy

Invited lecture

11:00 – 11:30 – **Dr. Genbo (Elvis) Xu, University of Southern Denmark, Denmark**

Beyond Size: Cross-Species Mechanistic Insights into Nanoplastic Toxicity and Future In Situ Imaging

11:30 – 11:50 – **Anna Zetterström, The University of Manchester, UK**

Microplastics accumulate in all major organs of the Mediterranean loggerhead sea turtle (Caretta caretta)

11:50 – 12:10 – **Karolina Kadela, NCSR Solaris, Jagiellonian University, Poland**

Exploring sub-zero behaviour of materials using O-PTIR

12:10 – 12:30 – **Prof. Peter Gardner, University of Manchester, UK**

Comparative Analysis of FTIR and OPTIR Spectra in Response to Fatty Acid Treatments and Hypoxia in PC-3 Prostate Cancer Cells

12:30 – 13:30 – Lunch

13:30 15:00 - **Session III:** applications of sub-micron IR spectroscopy

Invited lecture

13:30 – 14:00 – **Dr. Victoria Beltran, University of Antwerp, Belgium**

Coupling µFTIR and SR-µFTIR spectroscopy to OPTIR to unravel the composition of samples from polychromed layers from historical objects

14:00 – 14:20 – **Dr. Kaja Piana, NCSR Solaris, Jagiellonian University, Poland**

The nano-FTIR spectroscopy with synchrotron IR light setup at the CIRI beamline

14:20 – 14:40 – **Dr. Valeriia Skoryk, Lund University, Sweden**

High-resolution multimodal profiling of protein aggregates in CNS of Alzheimer's disease mouse models

14:40 – 15:00 – **Dr. Ferenc Borondics, SOLEIL, France**

Sub-micron infrared studies with synchrotron sources

15.00 – Poster session with coffee and fika; free discussion time

18:00 – Conference dinner at *Lundabryggeriets Ölkällare*,

Sankt Laurentiigatan 5A, Lund

Day 3 **Fri (2025-10-17)**

9:00 -10:30 – **Session IV:** applications of sub-micron IR spectroscopy

Invited lecture

9:00 – 9:30 – **Dr. Oxana Klementieva, Lund University, Sweden**

TBA

9:30 – 9:50 – **Tilda Sohlen, Royal Institute of Technology, Sweden**

Chemical imaging of amyloid plaques in 3D

9:50 – 10:10 – **Prof. Kajsa Uvdal, Linköping University, Sweden**

AFM-IR Imaging and PEEM reveal structural and chemical dynamics of immune cell activation

10:10 – 10:30 – **Dr. Xiaoni Zhan, Lund University, Sweden**

Strain-distinct α-Synuclein and Tau cross-seeding uncovered by correlative approach with O-PTIR sub-micron imaging

10:30 - 11:00 – Coffee break

11:00 - 12:30 – **Session V:** The future of sub-micron IR spectroscopy techniques

Invited lecture

11:00 – 11:30 – **Dr. Raul O. de Freitas, Brazilian Synchrotron Light Laboratory, Brazil**

LNLS synchrotron IR nanospectroscopy program: From Cells to Quantum excitations in 2D Materials

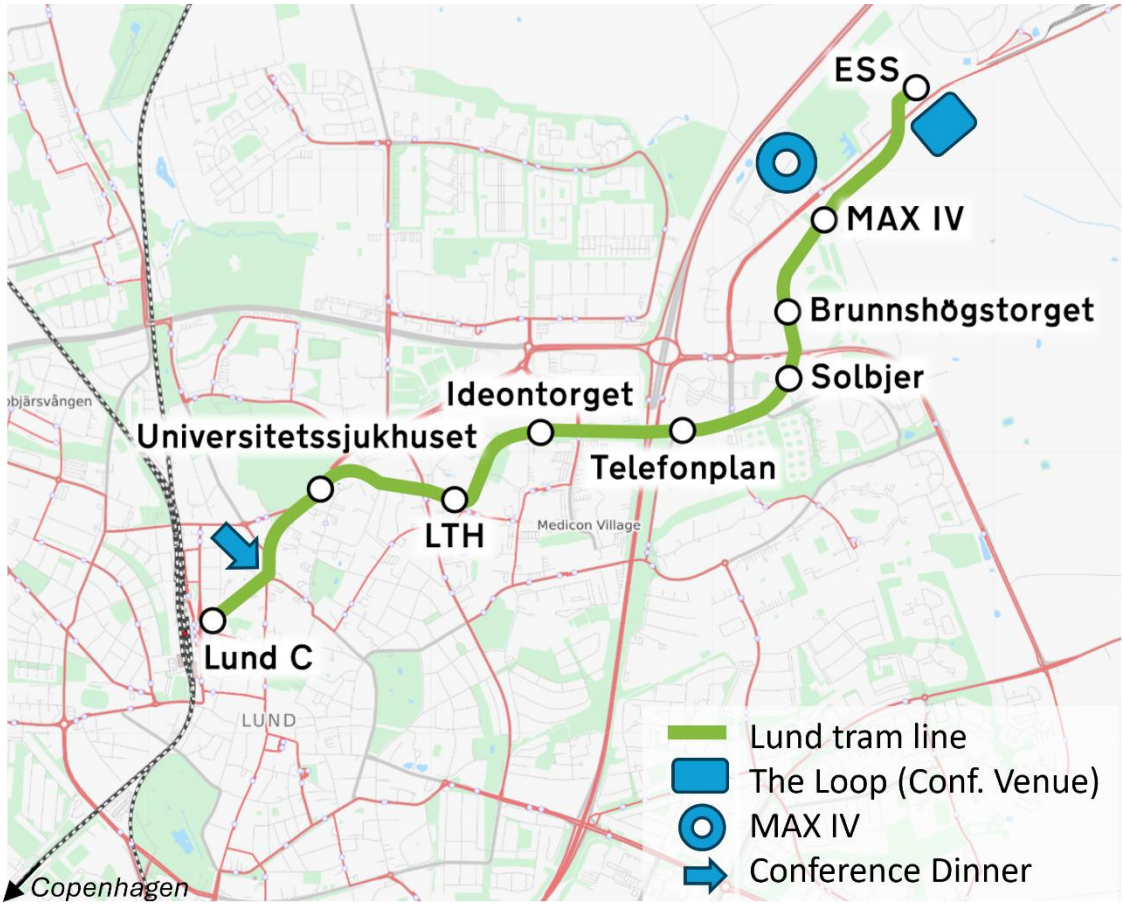
11:30 – 11:50 – **Dr. Nikolay Vinogradov, MAX IV Laboratory, Sweden**

MAX IV Joint Offline Lab for NanoIR Spectromicroscopy (MJOLNIR)

11:50 – 12:30 - Panel discussion: Future of sub-micron IR microscopy at MAX IV, the Nordics and beyond

12:30 – 13:30 – Lunch

14:00 – MAX IV visit (+ official inauguration of **MJÖLNIR,** the *MAX IV Joint Offline Lab for NanoIR Spectromicroscopy* at 15:00)



PRESENTATIONS – presenters in alphabetical order by first name, **invited** in bold

- Anna Zetterström - *Microplastics accumulate in all major organs of the Mediterranean loggerhead sea turtle (Caretta caretta)*
- Crislaine Fabiana Bertoldi - *Transforming microplastic analysis: the power of O-PTIR spectroscopy*
- **Elvis Genbo Xu** - *Beyond Size: Cross-Species Mechanistic Insights into Nanoplastic Toxicity and Future In Situ Imaging*
- **Ferenc Borondics** - *Sub-micron infrared studies with synchrotron sources*
- **Jeremie Mathurin** (for Alexandre Dazzi) – *Introduction and overview of AFM-IR spectroscopy*
- **Ji-Xin Cheng** (online) – *Optical Photothermal Infrared Microscopy: Innovations and Applications*
- Kaja Piana - *The nano-FTIR spectroscopy with synchrotron IR light setup at the CIRI beamline*
- Kajsa Uvdal - *AFM-IR Imaging and PEEM Reveal Structural and Chemical Dynamics of Immune Cell Activation*
- Karolina Kadela - *Exploring sub-zero behaviour of materials using O-PTIR*
- **Khaled Kaja** (for Hartmut Stadler) – *Practical AFM-IR*
- Maria Eleonora Temperini - *Multiscale IR Spectroscopy of Proteins at IRIS Beamline*

- **Miriam Unger** – *Practical O-PTIR*
- Nikolay Vinogradov - *MAX IV Joint Offline Lab for NanoIR Spectromicroscopy (MJOLNIR)*
- **Oxana Klementieva** - *TBD*
- Peter Gardner - *Comparative Analysis of FTIR and OPTIR Spectra in Response to Fatty Acid Treatments and Hypoxia in PC-3 Prostate Cancer Cells*
- **Raul Freitas** - *LNLS synchrotron IR nanospectroscopy program: From Cells to Quantum Excitations in 2D Materials*
- Szymon Tott - *Deep-dive into cell composition with O-PTIR in water environment*
- Tilda Sohlen - *Chemical Imaging of Amyloid Plaques in 3D*
- **Tue Hassenkam** - *NanoIR of biosignatures*
- Valeriia Skoryk - *High-resolution multimodal profiling of protein aggregates in CNS of Alzheimer's disease mouse models*
- **Victoria Beltran** - *Coupling µFTIR and SR-µFTIR spectroscopy to OPTIR to unravel the composition of samples from polychromed layers from historical objects*
- Xiaoni Zhan - *Strain-distinct α-Synuclein and Tau cross-seeding uncovered by correlative approach with Optical Photothermal Infrared Sub-Micron Imaging*

Microplastics accumulate in all major organs of the Mediterranean loggerhead sea turtle (Caretta caretta)

Leah Costello[1,7], Anna Zetterström[2,3*], Peter Gardner[2], Jose Luis CrespoPicazo[4], Cyrill Bussy[5,7], Ian Kane[6,7], Holly Shiels[1,7]

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[5]*Division of Immunology, Immunity to Infection and Respiratory Medicine, Faculty of Biology, Medicine and Health, The University of Manchester, Oxford Road M13 9PL, UK*

[6]*Department of Earth and Environmental Sciences, Faculty of Science and Engineering, The University of Manchester, Oxford Road M13 9PL, UK*

[7]*Manchester Environmental Research Institute, The University of Manchester, Oxford Road M13 9PL, UK*

Microparticles (MPs) are a pervasive environmental pollutant, posing a serious threat to marine life on all levels. Plastic ingestion is well documented in marine turtles, and loggerhead sea turtles (*Caretta caretta*) have been identified as an indicator species to monitor MP pollution globally. Our understanding of the translocation and bioaccumulation potential of MPs beyond the gastrointestinal tract is, however, limited. Here, we demonstrate that MP translocation occurs in these marine reptiles as accumulation in body tissues of 10 stranded Mediterranean loggerhead turtles was found in all major organs. Foreign microparticles were identified in 98.8% of all samples and were significantly concentrated in the reproductive organs followed by the heart. Optical Photothermal Infrared (O-PTIR) spectroscopy provides both the ability to identify microparticles and the spatial resolution to image foreign particles within tissue. Here, we present high resolution O-PTIR images identifying microparticles embedded in the tissue of loggerhead turtle hearts, proving its power for assessing microparticle bioaccumulation *in situ* [1].

References:

[1] Costello, L. *et al., Marine Environmental Research* 208, 107100 (2025)

Transforming microplastic analysis: the power of O-PTIR spectroscopy

Crislaine Bertoldi[1], Milda Pucetaite[2], Maria C. Hansson[1], Carl Troein[1], Martijn van Praagh[1,3]

[1] *Centre for Environmental and Climate Science, Lund University, Lund, Sweden*

[2] *Department of Biology, Lund University, Lund, Sweden*

[3] *Swedens Geotechnical Institute, Malmö, Sweden*

Microplastics are increasingly recognized as a pervasive environmental contaminant, with the application of biosolids as soil amendments representing a major pathway for their entry into terrestrial environments [1]. Their small size, persistence, and chemical leaching raise concerns for soil health, nutrient cycling, and potential uptake by organisms, yet their detection and characterization in such complex matrices remain analytically challenging. Conventional techniques such as μ-FTIR and Raman micro spectroscopy are limited by diffraction, scattering artefacts, and fluorescence interference, often excluding the smallest particles (<50 μm), which are also the most environmentally relevant. In this work, we demonstrate how optical photothermal infrared (O-PTIR) spectroscopy advances microplastic analysis in biosolids by combining sub-micron spatial resolution (~0.5 μm) with robust chemical specificity, surpassing the capabilities of both Raman and μ-FTIR [2].

With O-PTIR, we achieved reliable identification of fibers as thin as 2 μm and particles down to 5 μm, significantly surpassing the spatial resolution limit of μ-FTIR (~20 μm). Unlike Raman, O-PTIR spectra are absent from fluorescence interference, enabling more confident polymer identification even in coloured and complex samples. Single-frequency O-PTIR imaging also produced well-defined visualizations of particles embedded in biosolids, highlighting its potential for semi-automated microplastic mapping and quantification. In addition, spectral acquisition was faster when comparing both Raman and μ-FTIR.

However, certain limitations should be acknowledged. Morphological irregularities along the z-plane can present significant challenges during analysis. While the spectral range of 800– 1800 $cm^{-1}$is sufficient for identifying most common polymers, it may limit studies focused on degradation processes that require access to broader spectral regions, such as those above 3000 cm^{-1}. The potential for physical damage caused by laser power must also be taken into consideration. Additionally, the O-PTIR signal depends strongly on particle size, as smaller objects dissipate heat more rapidly, leading to a nonlinear photothermal response [2]. Acquiring multiple spectra from the same particle is therefore recommended to ensure reliable data.

Despite these challenges, O-PTIR represents a major step forward for high-resolution microplastic analysis in environmental samples. By overcoming long-standing technical limitations, O-PTIR establishes a new benchmark for environmental microplastic research. It expands the analytical window to the smallest microplastics, most likely to migrate into soil and interact with biota, supporting both fundamental science and future regulatory frameworks.

Keywords: microplastics, O-PTIR, biosolids, polymer identification

References:

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Beyond Size: Cross-Species Mechanistic Insights into Nanoplastic Toxicity and Future In Situ Imaging

'Elvis' Genbo Xu

Department of Biology, University of Southern Denmark, 5230 Odense, Denmark

Plastic pollution from microplastics and nanoplastics poses escalating ecological and health challenges, driven by their potential for systemic bio-interaction. While nanoplastics are often assumed to be more hazardous due to their small size and increased penetrability, the mechanistic basis for size-dependent toxicity across species remains unresolved. Here, we investigated nanoplastics (50 nm to 1000 nm) in two vertebrate models, zebrafish larvae (aquatic) and chicken embryos (terrestrial), during comparable developmental stages. Embryos were exposed to nanoplastics at concentrations of up to 10 ppm, with effects assessed via behavioural phenotyping, biochemical markers, RNA sequencing, and high- resolution 3D imaging.

Results revealed pronounced species- and size-specific responses: zebrafish displayed neurobehavioral hypoactivity and transcriptomic signatures of neurotoxicity, whereas chicken embryos exhibited structural malformations and extracellular matrix remodelling predominantly with larger particles. Additionally, both species exhibited conserved disruptions in hepatic and cardiovascular pathways, underscoring their multi-organ vulnerability. These findings challenge the prevailing "smaller-is-more-toxic" paradigm, emphasizing that NP risk profiles depend on both particle size and host biology. To overcome current limitations in real-time in situ visualization and biochemical mechanistic linkage, we plan to integrate miRage-LS, a next-generation sub-micron IR photothermal imaging system, for mapping the distribution of nanoplastics and associated biochemical alterations within transparent embryos. This approach will enable non-destructive, label-free tracking of particle fate and bio-interface changes, bridging a critical gap between exposure and phenotype. Our study not only advances comparative toxicology across taxa but also aims to set a new analytical frontier using miRage-LS to resolve nanoplastic–biological interactions at cellular and molecular scales in ecotoxicology.

Sub-micron infrared studies with synchrotron sources

Gergely Nemeth[1], Christophe Sandt[1], Francesco Capitani[1], Hans A. Bechtel[2], Ferenc Borondics[1]

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Both near- and far-field infrared microscopy are capable to reach spatial resolution below the micron scale. Sub-micron and sub-diffraction limit techniques have been important contributors to synchrotron studies in the past decade, with new opportunities to adapting recently rising techniques for the synchrotron source.

In this talk I will review some of the state-of-the-art capabilities around the world in and will give examples focusing on studies from the SMIS beamline in the SOLEIL synchrotron both from beamline staff and the user community. Finally, I will provide an outlook on recent developments that has the potential to revolutionize the field of synchrotron-based infrared spectromicroscopy.

Introduction and Overview of AFM-IR spectroscopy

Jeremie Mathurin[1], Alexandre Dazzi[1]

1 Institut de Chimie Physique, Université Paris-Saclay, CNRS, 91640 Orsay, France

The principle of AFM-IR technique is based on the coupling between a tunable infrared laser and an AFM (Atomic Force Microscope). The sample is irradiated with a pulsed nanosecond tunable laser. If the IR laser is tuned to a wavenumber corresponding to sample absorption band, the absorbed light is directly transformed into heat. This fast heating results in a rapid thermal expansion localized only in the absorption region detected by the AFM tip. Thus, the detection scheme is analogous to photo-acoustic spectroscopy, except that AFM tip and cantilever are used to detect and amplify the thermal expansion signal instead of a microphone in a gas cell. The thermal expansion induces cantilever oscillations that are rigorously proportional to the local absorption allowing to build up IR absorption spectra. These spectra use to correlate very well conventional IR absorption spectra collected by FT-IR spectroscopy. In addition, mapping oscillations amplitude versus tip position, for one specific wavenumber, gives a spatially resolved map of IR absorption that can be used to localize specific chemical functions[1]. Since the first proof of concept in 2005 [2], the AFM-IR technique has quickly evolved and is now applied from diverse research areas like materials science, life science, astrochemistry, and culture heritage [1], [3], [4].
After presenting a quick historical background of the AFM-IR technique, this presentation will focus on presenting the two main operating mode, the resonance-enhanced contact mode [5] and the tapping AFM-IR mode [6] and will present recent technical advancements and their use to study complex samples [7].

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[1] A. Dazzi and C. B. Prater, "*AFM-IR: Technology and Applications in Nanoscale Infrared Spectroscopy and Chemical Imaging*," Chem Rev **117(7)**, pp. 5146–5173 (2017), doi: 10.1021/acs.chemrev.6b00448.
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Optical Photothermal Infrared Microscopy: Innovations and Applications

Ji-Xin Cheng

Boston University, Boston, MA, 02215, USA

Abstract: Providing molecular fingerprint information, vibrational microscopy offers a platform to decipher the function of biomolecules in a living system. Classic vibrational microscopes based on spontaneous Raman scattering or mid-infrared absorption suffers from very small cross section or poor spatial resolution. Vibrational photothermal microscopy overcomes this daunting barrier and opens a new window to look at molecules with micromolar sensitivity and sub-micron resolution. In this method, a pump beam excites chemical bonds via mid-infrared absorption, stimulated Raman induced absorption, or shortwave infrared absorption. A probe beam measures the local change of refractive index or thermal expansion of a particle induced by the photothermal effect. Since the first demonstration of mid-infrared photothermal (MIP) imaging of living cells and organisms [1], our team has greatly advanced this pump-probe chemical imaging technology [2], including scanning confocal MIP microscopy till video rate [3], camera-based wide-field MIP microscopy [4], fluorescence-detected MIP microscopy [5], and photothermal reporters in silent window [6,7]. We have also developed computation-based MIP tomography [8]. More recently, we demonstrated stimulated Raman photothermal microscopy [9] and shortwave infrared photothermal microscopy [10] as new members of vibrational photothermal microscopy. Since the launch of mIRage in 2017, MIP microscope has been delivered to over 15 countries, enabling broad applications spanning the analysis of functional materials, characterization of viral particles and environmental microplastics, and structural detection of protein aggregation in neurological diseases.

References:

[1] Delong Zhang, Chen Li, Chi Zhang, Mikhail N. Slipchenko, Gregory Eakins, Ji-Xin Cheng, Depth-resolved mid-infrared photothermal imaging of living cells and organism with sub-micron spatial resolution, Science Advances, 2016, 2: e1600521.

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The nano-FTIR spectroscopy with synchrotron IR light setup at the CIRI beamline

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The Chemical InfraRed Imaging (CIRI) beamline of the SOLARIS synchrotron give an access to the users for three end stations, one of which is s-SNOM/AFM-IR end station equipped with neaSCOPE microscope. This end station was successfully coupled with the infrared (IR) beam coming from the synchrotron at the end of 2024. That enabled us to obtain first sets of the nanoscale Fourier transform infrared spectroscopy (nano-FTIR) spectra by detection of the tip-scattered synchrotron light. We observed that beam is not homogenous and depending on the alignment approach we can change the profile of the beam spectra. Especially, we observed higher intensity in the fingerprint region (500 cm^{-1} – 1100 cm^{-1} and 1280 cm^{-1} – 1490 cm^{-1}) than in others. Some example spectra of the beam profile will be presented. Moreover, the beam alignment aspects and optics enabling the propagation of the IR light from the synchrotron storage ring up to the end station will be shown.

This project is executed under the provision of the Polish Ministry and Higher Education project „Support for research and development with the use of research infrastructure of the National Synchrotron Radiation Centre SOLARIS" under contract no. 1/SOL/2021/2.

Participation in the First Nordic Sub-Micron IR Microscopy Conference - ECL and AIDA event has been supported by a grant from the National Synchrotron Radiation Centre SOLARIS under the Strategic Programme Excellence.

AFM-IR Imaging and PEEM Reveal Structural and Chemical Dynamics of Immune Cell Activation

Kajsa Uvdal

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Atomic force microscopy (AFM), infrared (IR) spectroscopy, and photoemission electron microscopy (PEEM) are widely used in surface and materials science to probe molecular vibrational modes, chemical and electronic states, chemical shifts, and work function profiles. Recent technological advances have extended the application of these techniques to nanomaterials and life sciences. By detecting local vibrational absorption, AFM-IR enables spatially resolved chemical mapping of proteins, lipids, nucleic acids, and other biomolecules with lateral resolution on the order of tens of nanometers, allowing direct correlation of chemical composition with subcellular structures.

In this project, we combine AFM-IR imaging with PEEM to visualize human neutrophil granulocytes during activation and in the presence of nanoprobes. Neutrophils exhibit a wide range of dynamic morphological states that reflect their maturation and activation pathways. Upon stimulation, they undergo rapid shape changes to spread and capture intruders and can release neutrophil extracellular traps (NETs), web-like chromatin structures decorated with antimicrobial proteins that immobilize and neutralize pathogens.

Using cryo-cut thin sections and intact whole-cell preparations, we reveal a new visualization mode that captures both intracellular organization and extracellular networks, with vibrational modes assigned to distinct cellular compartments. These results establish AFM-IR as a powerful nanoscale imaging method for mapping the local chemical landscape of cells and, in this study, for uncovering structural changes associated with the dynamic activation of immune cells.

Exploring sub-zero behaviour of materials using O-PTIR

Karolina Kadela[1,2,3]*, Karolina Kosowska[1], Szymon Tott[1], Tetiana Stephanenko[1,2], Maciej Roman[1], Tomasz P. Wróbel[1]

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Infrared (IR) spectroscopy is one of the most widely applied techniques for the characterization of materials, providing information on molecular vibrations within a sample. In recent years, significant progress has been made in the development of methods based on photothermal expansion detection, especially Optical Photothermal Infrared (O-PTIR) spectroscopy, which has attracted attention. In contrast to conventional Fourier Transform Infrared (FT-IR) microscopy, O-PTIR overcomes the diffraction limit, achieving submicron spatial resolution without the need for extensive sample preparation.[1,2]

To date, most studies using vibrational techniques have been carried out at room temperature (RT), or some experiments above RT conditions. However, the behaviour of materials at sub-zero temperatures has remained insufficiently explored. In this work, a temperature-controlled stage was integrated into the O-PTIR microscope, enabling spectroscopic investigations of thermally sensitive materials, such as triglycerides and polymers, at temperatures down to –100 °C. All measurements were performed in co- propagating mode using a 40x objective.

The experiments revealed a significant increase in O-PTIR signal intensity under cryogenic conditions, up to three times compared to room temperature. This enhancement improves spectral sensitivity, thereby facilitating in situ characterisation of thermosensitive samples. To further clarify the underlying mechanisms, systematic studies were conducted under varied experimental conditions, including changes in gaseous environment and substrate thermal conductivity. The experimental findings were supported by theoretical modelling, which allowed evaluation of the temperature dependence of the O-PTIR signal. The results contribute to filling the existing knowledge gap in low-temperature O-PTIR spectroscopy and highlight the potential of this technique for high-resolution studies of materials under cryogenic conditions.[3]

Acknowledgement(s): Measurements were performed at the CIRI beamline of the SOLARIS synchrotron facility under contract nr 1/SOL/2021/2. The work is funded by the Ministry of Higher Education and Science of Poland within the grant “Implementation Doctorate VII” no. DWD/7/0263/2023. Participation in the First Nordic Sub-Micron IR Microscopy Conference has been supported by a grant from the National Synchrotron Radiation Centre SOLARIS under the Strategic Programme Excellence Initiative at the Jagiellonian University.

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Multiscale IR Spectroscopy of Proteins at IRIS Beamline

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The recent upgrade with the scattering-type scanning near-field optical microscopy (s-SNOM) setup at the IRIS infrared (IR) beamline of the BESSY II storage ring [1] has extended the spatial resolution of IR spectroscopy to the nanoscale [2]. The experimental facilities available at the beamline enable characterization of materials on the milli- to nanometer scale. For biological materials this allows to obtain structural and chemical information from tissues down to subcellular level in the THz, far- and mid-IR spectral ranges. Here we give a brief overview of the IRIS beamline and capabilities of the available end-stations. To demonstrate the multiscale approach, we present our studies on α-synuclein fibrils, which are protein aggregates implicated in neurodegenerative disorders. Using nano-IR, we recorded mid-IR spectra from fibril bundles (20-30 nm thick) deposited on gold substrates, revealing that the characteristic cross-β absorption band shifts to lower wavenumbers when fibrils are formed in the presence of RNA (Fig. 1A-C) [3]. This spectroscopic signature, together with far-field micro-FTIR measurements and AFM topography analysis, indicates a reorganization of the supramolecular architecture, pointing to an RNA-mediated effect on protein aggregation pathways. A further step toward more native-like experimental conditions has been the development of dedicated in-liquid s-SNOM cells [4,5]. Preliminary measurements on α- synuclein fibrils under native-like aqueous conditions, using a SiN membrane, demonstrated the potential of this approach for nanoimaging and nanospectroscopy of protein aggregates (Fig. 1D-E), aiming to directly correlate nanoscale vibrational signatures with aggregation state and local environment. This research highlights the unique capabilities of the IRIS beamline to combine synchrotron brilliance with near-field IR microscopy, providing nanoscale chemical and structural insights into complex biological systems. Moreover, the extension of this study into the far-IR and THz range will enable the investigation of collective vibrational modes, opening new opportunities for studying the dynamics, interactions and functional properties of proteins and other biomolecules at the nanoscale.

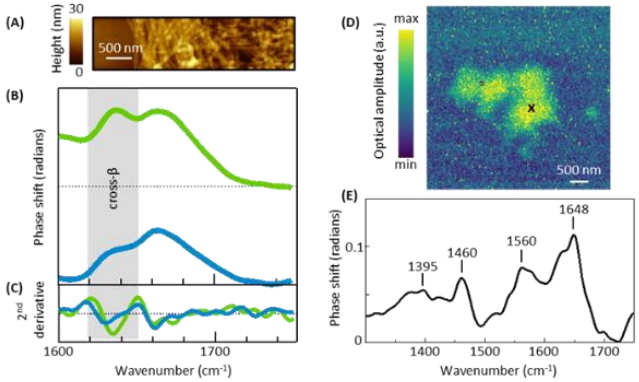

Figure 1. (A) Representative AFM topography of α-synuclein fibrils. (B) s-SNOM phase shift signal of α-synuclein fibrils alone (green) and co-incubated with RNA (blue). (C) Second order derivative of curves in (B). (D) s-SNOM optical amplitude of α-synuclein aggregates in solution. (E) s-SNOM phase shift signal acquired in the position marked in (D).

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MAX IV Joint Offline Lab for NanoIR Spectromicroscopy (MJOLNIR)

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The progress in making tuneable pulsed high-brilliance infrared sources – quantum cascade lasers and optical parametric resonators (QCL and OPO, respectively) made it possible to "hack" the diffraction limit in infrared microscopy and allowed for insights in submicron or even nanometer resolution. An optical photothermal infrared microscope (oPTIR) uses a green visible laser to locally probe the photothermal response of the sample, making it possible to perform imaging with chemical contrast or IR spectroscopy with resolution down to 400 nm. An atomic force microscope with infrared capabilities (AFM-IR) pushes this resolution further down to a few-nm, making possible imaging with an unprecedented detail level. In this contribution I'll give an overview of the newly opened user platform for high-resolution infrared spectromicroscopy – MJOLNIR – exemplified by some use cases and provide information on technical capabilities and limitations, as well as the access mode.

The official opening of MJOLNIR will take place on Friday 17th of October at 3 pm in MAX IV – WELCOME!

Comparative Analysis of FTIR and OPTIR Spectra in Response to Fatty Acid Treatments and Hypoxia in PC-3 Prostate Cancer Cells

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This study examines the effectiveness of Fourier Transform Infrared (FTIR) and Optical Photothermal Infrared (OPTIR) spectroscopy in detecting overall biochemical changes in PC- 3 prostate cancer cells treated with omega-3, omega-6, and combined omega-3/6 fatty acids under hypoxic conditions. FTIR, using Resonant Mie Scattering-Extended Multiplicative Scatter Correction (RMieS-EMSC), successfully identified broad biochemical trends but was affected by artifacts introduced during scatter correction. In contrast, OPTIR provided higher spatial resolution but had a smaller sampling area due to its point-by-point data collection, making it less effective in capturing broader biochemical patterns. Multivariate analysis of FTIR spectra revealed subtle biochemical effects of fatty acid treatments and hypoxia, while OPTIR did not detect these changes as clearly. Omega-3 treatment might be linked to protein stabilization and lipid organization, whereas omega-6 treatment might be associated with protein destabilization and lipid remodelling. Although FTIR and OPTIR provide complementary information, this study highlights the challenges in directly comparing the two techniques due to differences in resolution and sampling methods.

LNLS synchrotron IR nanospectroscopy program: From Cells to Quantum Excitations in 2D Materials

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Infrared (IR) spectroscopy is a cornerstone across disciplines—chemistry, materials science, biology, geoscience, cultural heritage, and energy—because it directly probes molecular bonds, phonons, carriers, and phase changes. Yet conventional IR microscopy is diffraction- limited; in the mid-IR this yields micrometer-scale lateral resolution, making it unable to resolve sub-micron heterogeneities such as organelles within cells, grain boundaries and domain walls, individual catalytic active sites, phase segregation in polymers, and excitations in 2D materials or ultrathin films.

To overcome this, LNLS operates a synchrotron-driven near-field platform (s-SNOM/nano-FTIR/SINS) that provides ~20–50 nm chemical and electrodynamic contrast, enabling studies from hydrated and fixed cells and bio-interfaces to complex oxides and polaritonic van der Waals crystals. Building on this foundation, the program now runs at the 4th-generation Sirius synchrotron via the IMBUIA beamline, delivering higher brightness, stability, and broadband coverage integrated with interferometric detection, fine environmental control and open-user mode, positioning LNLS to serve the community across multiple fronts and push nano-IR from cells to quantum excitations in 2D materials.

In this presentation, I will present highlights from more than ten years of the LNLS synchrotron IR nanospectroscopy program and outline future directions.

Deep-dive into cell composition with O-PTIR in water environment

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Optical Photothermal Infrared Spectroscopy (O-PTIR) has recently emerged as a new, easy-to-use spectroscopic tool for measurements of various biological systems at spatial resolutions up 30x better than conventional Fourier-transform IR (FT-IR) microscopy.[1] O-PTIR is a pump-probe system in which absorption of IR radiation from a quantum cascade laser (QCL) is detected by a second laser operating in the visible range. Right now, the experiments on the O-PTIR are done routinely only in the air with Cassegrain or refractive objectives, in both co-propagating and counter-propagating modes, and in the water in case of samples kept in between a glass slide and CaF2 window. [2,3]

Here we present our findings regarding various protocols for O-PTIR measurements of cells in the water, including, for the first time, with the use of 60x water dipping objective. The use of these objectives is highly desirable, as they simplify sample preparation and allow to image samples in higher spatial resolutions due to higher numerical apertures. The samples of cells from U2OS cell line and avian erythrocytes were measured in the air, in a "sandwich" configuration, with cells closed in between a glass and CaF_2 slides, and in a droplet of water. For the first time, we successfully acquired the O-PTIR spectra and images of cells with a water-dipping objective. Despite strong absorption of IR radiation by water measurements in yielded high quality spectra comparable to those measured in the air, as they allowed to use higher power of the probe laser. Some qualitative changes to bands of DNA, caused by hydration of the sample, were observed.

Acknowledgements

The work is supported under the Polish Ministry of Science and Higher Education project: "Support for research and development with the use of research infrastructure of the National Synchrotron Radiation Centre SOLARIS" under contract nr 1/SOL/2021/2

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Chemical Imaging of Amyloid Plaques in 3D

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In 2021, approximately 60 million people worldwide suffered from dementia, with the majority of cases attributed to Alzheimer's disease (AD), characterized by progressive cognitive decline and the pathological accumulation of amyloid-beta (Aβ) plaques. While Aβ deposition in the brain is well-documented, its presence and distribution in the spinal cord remain underexplored [1], [2].

In this study, mid-infrared photothermal (MIP) microscopy was employed to analyze formalin-fixed paraffin-embedded spinal cord tissue from three mouse genotypes: a healthy control (WT), a severely affected AD model (5xFAD), and a mildly affected TM3 model. Spectral analysis focused on the amide I region (1600–1700 cm^{-1}) [3], where secondary structural features of proteins were resolved.

Through second-derivative processing of hyperspectral images, minimal frequency shifts for β-sheets and α-helices were confirmed, enabling reliable reconstruction at fixed wavenumbers (1628 and 1656 cm^{-1}). The results demonstrate a clear increase in Aβ accumulation in diseased models, consistent with expected AD pathology, and validate MIP as a sensitive and label-free approach for detecting protein aggregation in complex tissues.

Aβ formation exhibits considerable morphological diversity where different plaque structures, including diffuse, dense, and cored forms, have been observed in varying proportions among patients. This variability has been suggested to reflect underlying differences in disease mechanisms, but it is essential to understand how polymorphic Aβ aggregates contribute to AD pathogenesis in the context of emerging Aβ-targeting therapies [4].

The ultimate goal of this work is to achieve 3D reconstructions of sections of mouse spinal cord of different genotypes in order to determine whether a dominant structure of Aβ plaques exists. For this, a mesoscope which is characterized by its large field of view and ability to accelerate large-scale imaging will be employed to enable efficient volumetric mapping of plaque architecture. These findings suggest that Aβ pathology extends beyond the brain to the spinal cord, highlighting the importance of investigating broader neuroanatomical regions in AD progression.

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NanoIR of biosignatures

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When analysing ancient carbonaceous material stored in small inclusions within old rock formations, a range of methods is needed to determine whether this material represents remnants of early life or merely abiotic deposits of carbon-rich matter. Traditionally, carbon isotope analysis and structural context have been the primary tools for inferring the origin of such material. However, we demonstrate that NanoIR, when combined with isotope analysis, provides much stronger evidence for a biotic origin of carbonaceous material. Additionally, we are investigating trace amounts of carbonaceous material preserved in meteorites to profile their composition.

High-resolution multimodal profiling of protein aggregates in CNS of Alzheimer's disease mouse models

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Early detection of amyloid plaques and protein aggregates with toxic potential is critical for improving diagnosis and prognosis of Alzheimer's disease (AD) as well as for understanding its pathology. However, current methods often miss complex structural details. This study explores the use of a multimodal imaging pipeline to detect and characterize extracellular and intracellular protein assembles in CNS of AD mouse models taking into account microenvironment conditions.

High-resolution X-ray phase-contrast tomography (XPCT), combined with optical photothermal infrared spectroscopy (OPTIR), provides label-free 3D imaging of protein structures at subcellular resolution (up to 500nm). We applied XPCT on brains and spinal cords from two AD mouse models — 5xFAD and hAPPNL-G-F knock-in. As a next step, we are acquiring an infrared profile from the same sample, which provides compositional data on lipid, nucleic acid and protein structures within extracellular and intracellular assembles. This is then followed by multiplex immunolabeling to bring compositional validation to the infrared and X-ray profiles of variative amyloid appearance and changes in surrounding tissue.

By incorporating all 3 state-of-the-art techniques, we observed accumulations of higher X-ray intensity voxels aligned with both increased and not increased intensity of infrared spectral peaks for ß-sheet, parallel and antiparallel structures. On the other hand, some immunolabeled extracellular and intracellular amyloid aggregates did not show change in X-ray data voxel intensity. Moreover, there were small protein aggregates that only partially overlapped with immunolabeling data. This workflow allowed the identification of different complex amyloid structures within 3D spatial context of surrounding microenvironment changes.

This novel multimodal approach enhances our understanding of amyloid composition and its toxicity by correlating it with changes in the microenvironment. By improving the detection of early Alzheimer's hallmarks, this method significantly advances the identification and characterization of potentially toxic amyloid species at disease onset.

Coupling µFTIR and SR-µFTIR spectroscopy to OPTIR to unravel the composition of samples from polychromed layers from historical objects

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Historical artifacts frequently contain polychromed layers composed of pigments bound within organic matrices. These layers are often extremely thin (typically <30 µm) and inherently heterogeneous, as they comprise both original materials and alteration products that accumulate over time, particularly at material interfaces. Discriminating between these compounds and mapping their spatial distribution is essential for reconstructing the objects' original composition and appearance, understanding ongoing degradation processes, and providing information on the appropriate conservation strategies.

Micro-Fourier transform infrared (µFTIR) spectroscopy in transmission mode provides high- quality data for identifying a wide range of cultural heritage materials, encompassing both amorphous and crystalline, organic and inorganic compounds. To achieve the spatial resolution needed for the study of thin polychromed layers, synchrotron radiation-based FTIR (SR-µFTIR) is often employed. More recently, optical photothermal infrared (O-PTIR) spectroscopy has emerged as a powerful technique thanks to its nanometric resolution, which allows the detection of smaller features.

Each technique has inherent limitations, including constraints on measurement time, signal- to-noise ratio, and potential radiation damage, as well as distinct sample preparation requirements. However, given the intrinsic heterogeneity of these materials, analysing different fragments can lead to non-comparable datasets. To address these challenges, we propose an integrated analytical workflow that combines µFTIR, SR-µFTIR, and O-PTIR on the same sample fragment.

In this presentation, we will highlight the potential of the proposed workflow together with the sample preparation strategies designed to meet the requirements of all three techniques, while ensuring compatibility with complementary analyses such as SEM-EDX and Raman spectroscopy. These strategies include the preparation of thin sections and the examination of small fragments using a diamond compression cell.

The application of this strategy will be illustrated through case studies. This will include the characterization of pigment particles (~5 µm in diameter) in oil paintings from Van Gogh and the detection of degradation processes at layer interfaces from historical altarpieces.

Strain-distinct α-Synuclein and Tau cross-seeding uncovered by correlative approach with Optical Photothermal Infrared Sub-Micron Imaging[1]

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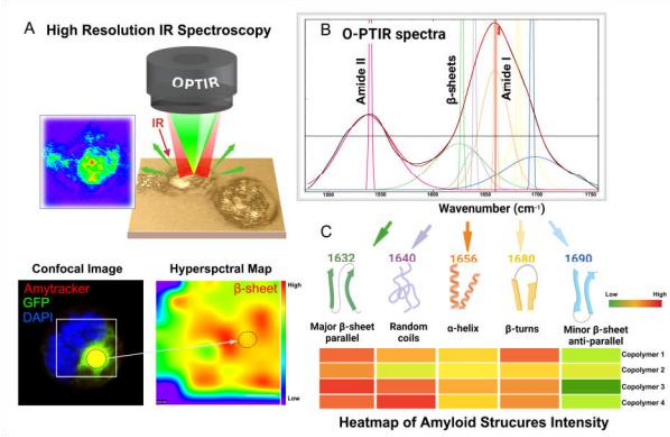
The co-occurrence of α-synuclein (αSyn) and Tau in synucleinopathies and tauopathies suggests a complex interplay between these proteins. Their cross-seeding enhances fibrillization, leading to the formation of diverse amyloid-specific structures enriched with β- sheets, which may influence their biological functions. However, existing tools cannot differentiate structural polymorphs directly in cells, as conventional microscopic approaches have limitations in providing structural insights into aggregates. As a result, a structurally relevant characterization of amyloids in their native cellular environment has not yet been achieved. In this study, we characterize the structural rearrangements of newly formed αSyn inclusions cross-seeded by different αSyn, and Tau preformed fibrils (PFFs) directly in cells, using a correlative approach that combines sub-micron optical photothermal infrared (O-PTIR) microspectroscopy and confocal microscopy. We found that hybrid PFFs synthesized from αSyn, and two Tau isoforms (Tau3R and Tau4R) exhibit variations in αSyn and tau composition. Specifically, structural polymorphs composed of αSyn and Tau3R exhibit the highest β-sheet content and most potent seeding potency, leading to enhanced phosphorylation within cellular inclusions. Importantly, we demonstrate that cellular inclusions inherit structural motifs from their donor seeds and exhibit distinct spatial and structural evolution. By providing subcellular-resolution structural imaging of amyloid proteins, our study uncovers divergent mechanisms of αSyn aggregation induced by αSyn/Tau PFFs in both mixed and hybrid formats.



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POSTERS – posters 1-7 are eligible for the Young Researcher poster prize

1. Mona Abbasi –
   The Colloidal State of Dissolved Organic Matter in Lakes and Its Significance for Recalcitrance
2. Åke Henrik-Klemens –
   Plasticizer Distribution and Interactions in the Pulp Cell Wall Revealed by O-PTIR and Solid-State NMR
3. Maria Lugojanu –
   Impact of ultrasonication on dsDNA: structural and stability changes after fragmentation
4. Honorata Oleś –
   Widefield Chemical Imaging with FL-PTIR: Tissue Analysis
5. Rimgaile Tamulyte –
   AFM-IR nanospectroscopy of S100 proteins on supported lipid bilayers in air
6. Dushyant K. Garg –
   Unveiling Pre-Condensate Nanoclusters as Key Determinants of TDP-43 LCD Assembly Pathways
7. Anna Zetterström –
   Preliminary investigation into multimodal imaging of renal tissue using infrared, Raman and mass spectrometry
8. Calley Eads –
   Sub-micron IR Microspectroscopy at MBIO
9. Leif Ericsson –
   NanoIR3 for Emerging Photovoltaic Materials at Karlstad University
10. Karolina Kosowska –
    What's the Key to High-Resolution Molecular Orientation Mapping? Developing a Robust Polarized O-PTIR Approach
11. Agnes Paulus –
    The Impact of Postmortem Delay on Amyloid Structures in Alzheimer's Disease: Insights from Optical Photothermal Infrared Microscopy
12. Milda Pucetaite –
    AFM-IR microspectroscopy of fungal-mineral interfaces
13. Ana Maria Labrador Garcia –
    Unleashing the power of HPC and Generative AI for Sub-Micron IR Microscopy: The FFplus Funding Calls
14. Carl Troein –
    CIPA and InfraVis

POSTER 1

The Colloidal State of Dissolved Organic Matter in Lakes and Its Significance for Recalcitrance

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Dissolved organic matter (DOM) is the largest pool of organic carbon in aquatic ecosystems, playing a critical role in global carbon cycling. DOM is operationally defined as the organic matter (OM) that passes through a commonly used 0.2 µm filter. Yet, it also contains a substantial colloidal fraction, comprising molecular aggregates and supramolecular structures at the sub-micron scale. The significance of this colloidal fraction for DOM persistence and degradation has received limited attention. In recent studies, colloidal DOM, extracted from a boreal forest soil, was characterized using scattering techniques and ^{1}H NMR [1], [2]. It was found that carbohydrates dominate the colloidal pool and that these structures are highly resistant to microbial decomposition, whereas truly dissolved molecules are rapidly degraded [3]. This suggests that the colloidal state is a key determinant of DOM recalcitrance. In this study, we aim to systematically characterize the contribution of colloids to the DOM pool, their role in resistance to bacterial degradation, and the molecular precursors of colloid formation across lake waters with different biogeochemical properties. Combining Infrared (IR) spectroscopy with scattering and NMR methods allows us to unravel the functional groups and chemical fingerprints of colloids. By applying this approach to water columns from a broad range of Swedish lakes, we connect colloidal chemical composition to size distributions and persistence. These findings will help clarify how the colloidal state influences DOM stability and its role in long-term carbon storage.

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POSTER 2

Plasticizer Distribution and Interactions in the Pulp Cell Wall Revealed by O-PTIR and Solid-State NMR

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The use of small organic molecules as plasticizers to modify the mechanical properties of pulp and paper has been of interest for decades; however, few studies have addressed the spatial distribution of these plasticizers within the pulp cell wall or identified the specific components they interact with. This gap in knowledge has hindered a comprehensive understanding of the precise role these compounds play in the thermoforming of pulp-based materials.

In this work, unbleached kraft pulp was plasticized with triacetylated glycerol (triacetin, TA) via water submersion. The interactions of the plasticizer in the pulp were analysed using polarization transfer and relaxation solid-state NMR (ssNMR). Additionally, the spatial distribution within the cell wall was mapped by analyzing cross-sections with the confocal vibrational spectroscopy technique optical-photothermal IR (O-PTIR). With ssNMR we found that the plasticizer was in contact with all the accessible components of the cell wall (cellulose, hemicellulose and lignin) and enhanced their mobility. O-PTIR detected TA in all parts of the cell wall, but at very uneven concentrations. O-PTIR was employed because the strong autofluorescence of lignin-rich pulp interfered with Raman microscopy; however, the high sensitivity of IR spectroscopy to carbonyl stretching significantly enhanced the study: by tracking the redshift of the ν(C=O) band of TA, it was possible to distinguish between TA in molecular contact with the cell wall and TA that was phase-separated. The combination of O- PTIR and ssNMR enabled complementary insights. First, the percentage of phase-separated lignin quantified by ssNMR could be spatially resolved using O-PTIR. Second, the distribution of TA throughout the fibre, as revealed by O-PTIR, supported the ssNMR findings that all accessible components of the pulp were in molecular contact with the plasticizer.

These findings support the thesis that the plasticizer acts both as a lubricant between components – reducing friction and easing sheer – and as a plasticizer, by dispersing molecularly in the wood-polymers themselves.

POSTER 3

Impact of ultrasonication on dsDNA: structural and stability changes after fragmentation

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Introduction: Rapid cancer detection relies on identifying circulating double-stranded DNA (dsDNA) fragments (120–220 bp) in plasma and widely investigated as a cancer biomarker [1]. Its concentration is significantly elevated in cancer patients compared to healthy individuals [2], but its short half-life (15–150 min) poses challenges for reliable detection. Cell- free DNA (cfDNA) is sensitive to pH, temperature, and mechanical stress, thus understanding its stability is crucial for biosensing applications. This study aims to evaluate how various ultrasonication times generate DNA fragments of different lengths and to investigate how fragmentation influences their structural integrity. Furthermore, the interaction of these fragments with two fluorescent dyes are assessed to gain insight into their binding behaviour and potential use for detection. Fluorescence quenching of Methylene Blue, which binds DNA through electrostatic and covalent interactions [3], was monitored upon DNA addition and MB–DNA complex formation confirmed by UV-Vis spectroscopy.

Results: Electrophoresis revealed minimal differences between the 30s and 40s fragmentation, both yielding DNA fragments around 400–500 bp. SG-bound DNA exhibited stable fluorescence across the tested pH range, however partial denaturation effects can be attributed to ultrasonication similar to extreme pH conditions. In the presence of MB, the fluorescence intensity decreased with increasing DNA concentration, indicating binding through electrostatic interaction and intercalation of the dye into the double helix of the DNA. The obtained calibration curve showed a linear correlation ($R^2 = 0.986$) between the mass of 30 s sonicated fragmented DNA and normalized the MB fluorescence signal, supporting its potential use as a quantitative assay for fragmented DNA. UV-Vis analysis showed that MB absorbance decreased with DNA mass for both genomic and fragmented samples. However, only control dsDNA caused a 7 nm red shift in MB's absorbance peak, suggesting the formation of a more extensive MB–DNA complex of the control DNA compared to that with fragmented DNA.

Conclusions: Ultrasonication effectively generates DNA fragments across a range of lengths around 400–500 bp. The size of DNA fragments influences their interaction with dyes under various pH conditions. SybrGreen serves as a sensitive probe for structural integrity of dsDNA, while Methylene Blue fluorescence can be used both to probe binding mechanisms and to quantify DNA concentration. These results provide insights into the stability of fragmented DNA and suggest that combining results from SybrGreen and Methylene Blue tests could enhance their potential as dye-based direct DNA detection platforms.

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POSTER 4

Widefield Chemical Imaging with FL-PTIR: Tissue Analysis

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Fluorescence Detected Photothermal Infrared (FL-PTIR) spectroscopy is a modern chemical imaging technique that combines infrared light absorption with the detection of changes in fluorescence intensity. The principle relies on a local change in sample temperature caused by the absorption of pulsed IR laser light, which leads to variations in fluorescence emission and enables the recording of absorption maps in the infrared range. As a result, FL-PTIR allows fast, wide-field imaging with high spatial resolution, far beyond the diffraction limits of traditional infrared spectroscopy. This technique makes it possible not only to acquire fluorescence images and infrared absorption maps, but also to obtain complete absorption spectra for every pixel. In turn, this opens the way to hyperspectral data acquisition and molecular distribution mapping on the nanometer scale. The advantages of performing measurements with this method also arise from the possibility of exploiting autofluorescence present in many biological samples, such as collagen, elastin, or chlorophyll in plants. Autofluorescence eliminates the need for external dyes or labels, making the measurements minimally invasive, suitable for live samples, and reducing the risk of altering biological structures.[1,2]

These studies demonstrate the potential of this technique when combined with PCA-based denoising and chemometric analysis, enabling chemical characterization of samples such as mouse liver tissue or human breast cancer tissue microarrays (TMAs). The ability to measure the decrease in fluorescence over time also allows for mathematical correction of photobleaching of the results, which enables proper analysis and obtaining reliable data. The obtained results demonstrate the significant potential of the method for diagnostic applications, as well as for the study of diseases at the subcellular level.

Acknowledgement(s): Measurements were performed at the CIRI beamline of the SOLARIS synchrotron facility under contract nr 1/SOL/2021/2. Participation in the First Nordic Sub-Micron IR Microscopy Conference has been supported by a grant from the National Synchrotron Radiation Centre SOLARIS under the Strategic Programme Excellence Initiative at the Jagiellonian University.

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POSTER 5

AFM-IR nanospectroscopy of S100 proteins on supported lipid bilayers in air

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The aggregation of S100-family proteins at lipid membranes plays a critical role in bilayer destabilization, contributing to neuronal damage in neurodegenerative diseases like Alzheimer's. It is known that the physicochemical properties of lipid membranes, such as charge, fluidity, and domain organization, can significantly influence protein adsorption and conformational transitions. However, a detailed understanding of how these factors modulate S100 structure and function at the membrane interface is lacking.

This study applies top-down AFM-IR to co-register morphology and vibrational contrast of S100A8, S100A9, and the S100A8/A9 heterocomplex on solid-supported lipid bilayers (SLBs) prepared in air and stabilized with trehalose. Three membrane systems were examined without calcium: (i) anionic DOPC/DOPE/DOPS/Chol with S100A8, S100A9, and S100A8/A9; (ii) brain total lipid extract with S100A9 and S100A8/A9; and (iii) neutral DOPC/Chol with S100A9. Hyperspectral maps (800–1800 cm^{-1}) targeted protein amide I/II and lipid ester C=O vibrations to quantify composition-dependent adsorption and secondary- structure markers.

Spectra consistently exhibited an amide-I spectral band dominated by disordered/α-helical signatures with some β-sheet contributions. Preliminary spatial analysis reveals protein-rich domains. Anionic SLBs supported stronger protein signals than neutral DOPC/Chol, while brain extract bilayers displayed distinct spectral contrasts consistent with compositional complexity. Together, these results demonstrate that AFM-IR mapping resolves nanoscale variations in S100 secondary structure and membrane response across physiochemically distinct bilayers in air-fixed membrane. Ongoing work includes quantitative band-shape deconvolution of amide I, peak-position and integral-intensity mapping, and correlation with topography to establish structure–function relationships for S100A8/A9 at charged and neutral interfaces.

POSTER 6

Unveiling Pre-Condensate Nanoclusters as Key Determinants of TDP-43 LCD Assembly Pathways

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Biomolecular condensation can organize macromolecules like proteins and nucleic acids into a dense, droplet-like phase (condensates) and a dilute phase. Elucidation of the condensate formation pathways is difficult due to limited information about the intermediates formed in the transition from monomers to droplets. According to classical nucleation theory when macromolecules reach a specific saturation concentration (Csat), they form condensates in one-step process. However, this framework does not explain the inherent heterogeneity in the condensates as-well-as the formation of diverse assembly products like gel, amyloid, etc.

Previously, we found that the low-complexity domain of TDP-43 (TDP43-LCD) gradually forms gels at pH 6 over 48 hours, while it forms liquid-like droplets instantly at pH 7. Notably, TDP43-LCD does not form droplets in the gelation regime at pH 6, even at concentrations 50 times its Csat at pH 7. Here, we report that TDP43-LCD exists as heterogeneous clusters sized between 50 and 200 nm, as shown by dynamic light scattering, super-resolution microscopy, and electron microscopy. Depending on the solution pH, these flexible nanoclusters can undergo different phase transitions, such as gelation or condensation. Testing condensate-promoting (G335A) and condensate-disrupting (A326P & W334G) mutants revealed that they also formed dynamic nanoclusters with varied sizes and topologies. These mutants produced amyloid aggregates at pH 6 without forming droplets.

We propose that the properties of these nanoclusters, including their size, charge, and monomer chain conformation, influence their phase behavior. High pH or salt conditions neutralize their charge, causing them to quickly collapse into droplets and subsequently to amorphous aggregates. In contrast, a highly charged environment (lower pH) increases their solubility, promoting slow interactions that facilitate their ordered assembly. We suggest that these nanoclusters are kinetically trapped entities whose assemblies can explain various phase transitions, such as gelation, amyloid aggregation, and different condensate features, including hollow condensates.

POSTER 7

Preliminary investigation into multimodal imaging of renal tissue using infrared, Raman and mass spectrometry

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Chemically specific imaging techniques, such as vibrational spectroscopy and mass spectrometry imaging (MSI) applied to biological tissue have seen an increasing interest in recent years. Multimodal imaging combining these techniques across spatial scales generates complementary information, promising a better understanding and explainability of the chemistry of the tissue [1]. In this work we have used both vibrational spectroscopy and mass spectrometry-based modalities to provide chemical maps ranging from the micron to sub- micron scale on renal cancer tissue. Fourier-transform infrared (FTIR) imaging and quantum cascade laser infrared (QCL-IR) imaging enable rapid, label-free assessment of broad chemical distributions at micron resolution, while optical photothermal infrared (O-PTIR) and stimulated Raman scattering (SRS) imaging provide sub-micron spatial resolution. These vibrational techniques are complemented by desorption electrospray ionization mass spectrometry imaging (DESI-MSI), which delivers molecularly specific information on lipids, metabolites, and other small molecules from the tissue, but at significantly poorer spatial resolution. See Fig 1. Here we discuss the advantages and disadvantages of the techniques and this multimodal approach and discuss the challenges associated with sample preparation and common substrates.

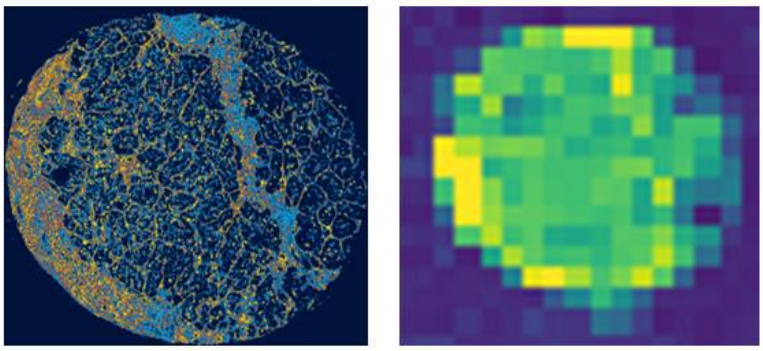

Figure 1. *Left: O-PTIR image of renal tissue core imaged at 0.5 µm resolution. Right: DESI image of renal tissue core imaged at 75 µm resolution.*

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POSTER 8

Sub-micron IR Microspectroscopy at MBIO

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Researchers at the Microscopy for Biosciences (MBIO) facility, a Faculty of Science infrastructure platform at Lund University, apply sub-micron IR microspectroscopy techniques (O-PTIR, AFM-IR) to investigate nanoscale chemical changes in biological systems. For instance, to explore the role of fungi in complex soil ecosystems, researchers study individual fungal hyphae on different mineral surfaces that mimic soil nutrients to disentangle the interaction mechanisms via exudates surrounding the hyphae using O-PTIR and, more recently, AFM-IR.

Other research projects focus on biomedical applications, such as using tissue sections and whole cell nanoscale chemical imaging to discriminate between protein aggregates linked to neurodegenerative diseases. Sub-micron IR methods are also advancing studies of micro- and nanoplastics in soil and biomass samples, providing new insights into their composition and distribution. O-PTIR and AFM-IR are becoming essential tools for supporting diverse biological research at MBIO.

In close collaboration with MAX IV, these techniques also serve as preliminary and complementary approaches to X-ray imaging beamlines such as MAXPEEM, NanoMAX and SoftiMAX. In my role as research engineer at MBIO, I work closely with users to support both instruments and experimental workflows and will showcase the facility's capabilities through examples ranging from sample preparation to instrument specifications and scientific applications such as those described above.

POSTER 9

NanoIR3 for Emerging Photovoltaic Materials at Karlstad University

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At Karlstad University (KaU) we have since 2019 a nanoIR3 system from Bruker/Anasys Instruments installed. Our main research performed in the nanoIR3 concerns thin films for organic solar cells and perovskite based solar cells.

Organic Photovoltaic (OPV) devices are often based on a nanostructured morphology of donor-acceptor blend films, crucial for the performance of OPV. Materials for both fullerene containing, and non-fullerene acceptor OPV cells are studied in research projects at KaU, aiming for a better understanding of film formation as well as degradation processes. Also, metal halide perovskite films are studied with the goal to understand their degradation processes.

Most well-known characterization techniques, such as scanning probe and electron microscopies, do not provide the chemical contrast and nano-scale resolution to map the distribution of donor and acceptor molecules in OPV blend films. Numerous studies of nanostructured donor-acceptor blend films by scanning probe microscopy techniques have resulted in surface topography images without resolving the actual distribution of donor and acceptor molecules. Non-destructive, high-resolution imaging techniques are needed to resolve the fine nanostructure in OPV blend films. AFM-IR spectromicroscopy combines the high resolution of atomic force microscopy with the chemical fingerprint of infrared spectroscopy.

The nanoIR3 combines the high resolution of scanning probe microscopy with the chemical fingerprint of infrared spectroscopy. Using a pulsed, tuneable MIRcat IR laser in the 900 - 1900 cm^{-1} range, tapping mode AFM-IR yields compositional maps of donor and acceptor molecules in OPV blend films based on their specific IR fingerprints.

Some examples from our research are shown. We demonstrate the presence of PC70BM network with characteristic length of 20 nm inside micrometer sized phase-separated domains of a donor:fullerene blend. Non-fullerene acceptor blend films for OPV were mapped in great detail revealing fine fibrils in the polymer acceptor-rich phase of an all-polymer blend. Furthermore, we show examples where AFM-IR could reveal changes in metal halide perovskite films upon degradation in air.

The results demonstrate the potential of AFM-IR as a high-resolution and non-destructive chemical analysis technique for emerging photovoltaic materials. Examples of results as well as some lessons learned in using AFM-IR are shown.

POSTER 10

What's the Key to High-Resolution Molecular Orientation Mapping? Developing a Robust Polarized O-PTIR Approach

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In recent years, O-PTIR microscopy has gained popularity, especially in studies involving biological systems and polymers. This technique offers superior spatial resolution compared to traditional FT-IR microscopy, and the sample preparation is less time-consuming. Accurately identifying molecular orientation at high spatial resolution is essential for deepening our understanding of key processes in organic systems, such as disease progression, tissue degeneration, and how structural features relate to material properties. Through the use of polarized O-PTIR microscopy, it is possible to acquire insights into the three-dimensional orientation of molecules and the extent of their self-organization at the submicron scale. The method developed for calculating of 2D and 3D angular orientation is both thorough and easily applicable to a variety of sample types, including biological specimens like tissues [1] and polymer materials [2], [3]. In the field of materials science, advancements in O-PTIR (fluorescence, wide-filed) microscopy have opened new avenues for investigating critical phenomena like the diffusion of nanonucleating agents in polymers during crystallization and unexpected moving of modifires in composites. The integration of polarized IR microscopy with fluorescence has enabled direct observation of phenomena such as the self-assembly of polylactide macromolecules in the presence of labeled nanoadditives, the migration behavior of them, and interactions occurring at phase boundaries.

Acknowledgments:

This research was supported by the National Science Centre, Poland (SONATINA 7, "Study of the effect of modifiers on the crystallization process of thermoplastic polymers: polarized IR microscopy below the diffraction limit", Grant. No. 2023/48/C/ST4/00176). Measurements were performed at CIRI beamline under the provision of the Polish Ministry and Higher Education project support with the use of research infrastructure of the NCPS SOLARIS under contract nr 1/SOL/2021/2.

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POSTER 11

The Impact of Postmortem Delay on Amyloid Structures in Alzheimer's Disease: Insights from Optical Photothermal Infrared Microscopy

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The accumulation of amyloid proteins characterizes Alzheimer's disease (AD); however, the effects of postmortem delay (PMD) on these protein structures are still poorly understood. This study investigates how PMD affects amyloid organization using Optical Photothermal Infrared (OPTIR) microscopy, a high-resolution, label-free technique, alongside traditional biochemical methods, such as immunolabelling.

Brain tissue from 8-month-old transgenic AD mice and wild-type controls was analyzed at PMD intervals of 0, 6, and 24 hours. Initial findings suggest that PMD significantly alters amyloid structure: after 6 hours, amyloid proteins in AD mice resemble, indicating early degradation or structural rearrangement. However, by 24 hours, stabilization occurs, with amyloid structures regaining antiparallel beta-sheet characteristics. These results highlight the dynamic nature of amyloids in postmortem tissue and stress the importance of considering PMD in both experimental and clinical research. By refining tissue-handling protocols, this study enhances the reliability of AD investigations and may contribute to more accurate diagnostic approaches and therapeutic strategies targeting amyloid aggregation.

Keywords: Alzheimer's disease, postmortem delay, infrared spectroscopy, amyloid structure

POSTER 12

AFM-IR microspectroscopy of fungal-mineral interfaces

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Soil fungi play an important role in biogeochemical cycles via mineral weathering, organic matter (OM) decomposition and contributions to formation of organo-mineral complexes in soil. To better understand these processes, we have previously used soft X-ray scanning transmission X-ray microscopy in combination with near-edge X-ray absorption fine structure spectroscopy (STXM-NEXAFS) at the C(K) and Fe(L) absorption edges to study fungal- mineral interfaces [1]. We found that exudates of the symbiotic fungus *P. involutus* which deposit around the soil mineral goethite contain organic substances, which cause reduction of Fe in the mineral. Mineral weathering taking place at the sites of Fe reduction is key for subsequent formation of organo-mineral interfaces and, thus, carbon storage in soils [2]. While STXM-NEXAFS allowed us to observe fungal-mineral interactions at micro- to nanoscale for the first time, the use of molecular-composition-sensitive technique such as AFM combined with infrared (AFM-IR) spectroscopy can provide more extensive information on the molecular chemistry and chemical responses of the exudates.

Here we show that AFM-IR spectroscopy can be used to trace both topography and chemistry of hyphal exudates of saprotrophic soil fungus *Psilocybe cf. subviscida* grown on mineral muscovite surface at nanometer scale. We were able to record high quality single IR spectra, multispectral maps and single-frequency images of selected areas on the hyphal tips - functionally most active part of the hyphae. We found that the main constituent of the exudate layers of *P. cf. subviscida* are carbohydrates, likely sugars, which is in line with our previous results obtained via STXM-NEXAFS [1]. While further experiments comparing the hyphal- mineral interactions across different fungal species and functional groups grown on different mineral surfaces are necessary, at a larger perspective, such knowledge can aid in uncovering the mechanisms of biological mineral weathering and physical carbon stabilization through formation of organo-mineral interfaces. The latter is crucial to identify soil cultivation techniques which foster this process, and to secure soil fertility and increase the carbon sink potential of our soils.

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POSTER 13

Unleashing the power of HPC and Generative AI for Sub-Micron IR Microscopy: The FFplus Funding Calls

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High-performance computing (HPC) and artificial intelligence (AI) are rapidly becoming essential technologies to accelerate progress across practically all fields — from social, administrative, and business sectors to cutting-edge scientific research. Their impact is particularly visible in domains where technological complexity and data volume are rapidly increasing.

High-resolution imaging is one such domain. Modern techniques generate vast and intricate datasets, requiring sophisticated workflows for data processing, analysis, and integration, as well as driving the development of more advanced instruments.

The Fortissimo Plus (FFplus) project [1] provides a European framework that empowers small and medium-sized enterprises (SMEs) and startups — often in collaboration with researchers — to access HPC and AI resources (*Fig 1.*) to solve their business challenges. Through open calls for *innovation studies* and *business experiments* (*Fig 2.*), FFplus provides funding to lower HPC adoption barriers and to foster the development of new solutions, applications, and technologies [2]. Building on a history of success stories in diverse fields, like *HPC-enabled microscopy* [3], FFplus continues to demonstrate how advanced computing can accelerate innovation and enable the uptake of HPC and generative AI as a new level of digital capability.

My participation at this conference, as FFplus Coordinator at Galicia Supercomputing Center [4] (CESGA), is part of the FFplus project's outreach, aimed at exploring synergies that promote cross-disciplinary innovation between the research community and digital infrastructures.

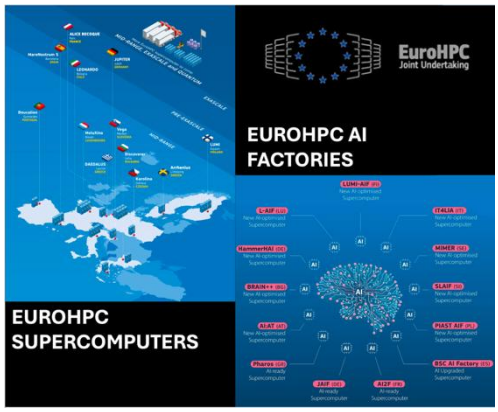

Fig. 1 European HPC and AI Factories.

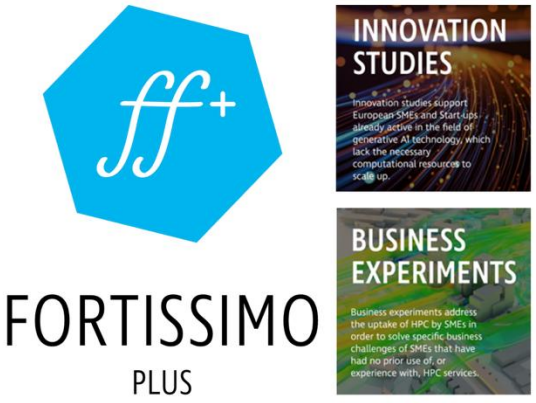

Fig. 2 FFplus Business Experiments and Innovation Studies.

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POSTER 14

CIPA and InfraVis

Carl Troein[1,2], Jonas Ahlstedt[1,2], Alexandros Sopasakis[1,2], Emanuel Larsson[1,2], Kajsa M. Paulsson[1,2]

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[2] *InfraVis National Research Infrastructure, infravis.se*

CIPA[1] is a Lund University research infrastructure for management, analysis and visualization of scientific data. The main motivation for CIPA is the amount of expertise needed to handle the complexity and volume of modern imaging data. CIPA mainly provides access to expertise, but also to computer hardware and imaging software.

InfraVis[2] is the Swedish national research infrastructure for data visualization. InfraVis helps researchers visualize research data gives access to state-of-the-art visualization competence, support, equipment, training, and methods.

See our poster and websites to learn more about what we can do for you. You are warmly welcome to attend the monthly CIPA drop-in sessions at BMC (see cipa.lu.se for dates)

References:

[1] CIPA Website: www.cipa.lu.se

[2] InfraVis Website: www.infravis.se ..

Alphabetical (on last name) list of participants

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