Illuminating Biomolecular Complexity: X-ray Free Electron Lasers and Vibrational Spectroscopies for Protein, Aggregates, and Cellular Architectures

Report of Contributions

Contribution ID: **2** Type: **Contributed Talk (≈20 minutes)**

Picosecond X-ray pulses at Elettra 2.0 with crab cavities

Picosecond-long x-ray pulses of moderate intensity and up to MHz CW repetition rate for time-resolved analysis of matter in the linear response regime are proposed for un upgrade operation of Elettra 2.0, now in construction as funded successor of the Elettra storage ring light source in Trieste, Italy. The scheme, based on the adoption of radiofrequency transverse deflecting cavities, promises a spectral flux at 1–10% level of the standard single bunch emission at the sample, transverse coherence in both transverse planes up to 0.5 keV photon energy, and it turns out to be simultaneous and largely transparent to the standard multi-bunch operation. The project well matches the view of an integration of storage ring and free electron laser communities, viewing their co-location as a crucial asset for advancing time-resolved science.

Scholarship elegibility

no

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Contribution ID: **3** Type: **Contributed Talk (≈20 minutes)**

X-ray Emission Spectroscopy for Real-Time Diagnostics in SFX experiments: A Machine Learning Approach

X-ray emission spectroscopy (XES) complements structural techniques like serial femtosecond crystallography (SFX) by providing insights into the electronic states at specific sites within a sample. At X-ray free-electron lasers, simultaneous SFX and XES measurements using a single pulse have already been performed —such as the determination of the oxidation states in metalloproteins. By using non-thermal plasma simulations alongside relativistic atomic data, we trained a neural network on synthetic XES data from protein crystals to predict fluence and pulse duration of the beam. Trained on synthetic data generated by a collisional radiative model, the network accurately predicts fluence with <1.5% relative error and when predicting both parameters concurrently with <12% error. Feature importance analyses reveal spectral regions tied to underlying physical mechanisms. The model emphasizes K to L shifts to higher emission energies due to presence of highly charged sulfur ions. This approach performs comparably to, and in some cases better than, current experimental setups that rely mainly on upstream X-ray gas monitors (XGMs). It offers a promising route toward real-time, high-repetition-rate diagnostics, effectively complementing existing XFEL beam characterization methods.

Scholarship elegibility

no

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Contribution ID: **4** Type: **Contributed Talk (≈20 minutes)**

Low background high-repetition rate 3D X-ray imaging of single bio-particles using a helium-electrospray.

Imaging the structure and observing the dynamics of isolated proteins using single-particle X-ray diffractive imaging (SPI) is one of the potential applications of X-ray free-electron lasers (XFELs). Currently, SPI experiments on isolated proteins are limited by three factors: low signal strength, limited data and high background from gas scattering. The last two factors are largely due to the shortcomings of the aerosol sample delivery methods in use. Here we present our modified electrospray ionization (ESI) source, which we dubbed helium-ESI (He-ESI). With it, we decreased the gas load in the interaction chamber corresponding to an 80% reduction in gas scattering when compared to the original ES and increased particle delivery into the interaction region by a factor of 10, for 26 nm-sized biological particles. The increased particle delivery was measured using light scattering and also to measure the size and location of single viruses and protein complexes forming an aerosol beam. We were able to detect individual particles down to 16 nm in diameter. The primary purpose of our scattering instrument is to monitor the delivery of single bioparticles to the focus on an X-ray laser and using the He-ESI to potentially increase the quality and quantity of SPI diffraction patterns in future experiments resulting in higher-resolution structures.
In November 2023 we performed an SPI experiment at the SQS endstation on various samples based on low gas background gas scattering. We reduced the background from the gas scattering by a factor of ~ 5 and obtained many diffraction patterns from Bacteriophage MS2, a small virus. Most significantly, we have collected the first dataset of a protein complex, Photosystem I, an important membrane protein, by X-ray SPI. The recorded diffraction patterns match that of photosystem I and we estimated a resolution of 6 nm by phase retrieval transfer function.

Scholarship elegibility

no

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Contribution ID: **5** Type: **Flash talk (≈5 minutes)**

MS SPIDOC: Coherent diffractive imaging of proteins and viral capsids

MS SPIDOC is an innovative sample delivery system tailored for single-particle imaging at X-ray Free-Electron Lasers (XFELs) and adaptable to most large-scale facility beamlines. It accommodates a wide range of biological samples, from small proteins to megadalton (MDa) complexes. Utilizing nano-electrospray ionization, ionic samples are m/z-filtered and structurally separated before reaching the interaction zone for imaging. We present the first proof-of-principle experiments demonstrating gas-phase small-angle X-ray scattering (SAXS) at the PETRA III synchrotron (DESY, Germany), highlighting the system's potential for advancing structural biology in the gas phase.

Scholarship elegibility

no

Primary author: KIERSPEL, Thomas

Presenter: KIERSPEL, Thomas

Contribution ID: **6** Type: **Contributed Talk (≈20 minutes)**

Nanospectroscopy Study of Amyloid Aggregates Interacting with RNA

Studying structural changes associated with protein aggregation is challenging and often requires a combination of experimental techniques to capture insights at the molecular level across different scales, from nanometers to microns. Studying this process becomes even more complex when aggregation occurs in the presence of molecular co-factors, nucleic acids among them, and when the resulting aggregates exhibit a high structural and morphological polymorphism. Here, we investigate the potential structural effects of RNA on amyloid protein fibrils. To achieve this, infrared (IR) spectroscopy, known for its high sensitivity to structural changes in the cross-β architecture of protein aggregates, was employed. In particular, IR spectroscopic analysis was performed by combining Fourier transform infrared (FTIR) microspectroscopy (micro-FTIR) and IR nanospectroscopy approaches relying on the use of an atomic force microscope (AFM) to probe the supramolecular architecture of aggregates at the nanoscale. Co-incubation with RNA was shown to alter the α-synuclein (α-syn) fibril architecture by promoting the formation of more rigid fibrils and to reduce the structural polymorphism within the fibril population. Additionally, AFM morphological characterization on individual α-syn fibrils demonstrated that RNA modifies the morphological properties of fibrils, reducing their diameter and increasing their persistence length. Remarkably, IR nanospectroscopy experiments demonstrated that RNA had a more pronounced impact on the supramolecular architecture of α-syn ordered fibrils compared to less ordered amyloid aggregates, suggesting that RNA has distinct structural effects depending on the aggregate architecture. This finding suggests that RNA may have varying interaction affinities for different types of aggregates, leading to distinct modifications in their supramolecular architectures depending on their structural organization.

Scholarship elegibility

no

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Contribution ID: **7** Type: **Contributed Talk (≈20 minutes)**

Single particle imaging of biomolecules using Coulomb Explosions.

Single particle imaging of biomolecules using Free electron lasers (FEL) is an imaging technique that has been under development since the dawn of FEL:s more than two decades ago. Due to the heavy ionisation, biomolecules exposed to FEL pulses explode. In a recent publication (Phys. Rev. Lett. 134, 128403 (2025)) we have described how we can harvest information about the molecular structure of protein, solely but measuring the ions ejected from the explosion. In this simulation study we were able to separate protein structures that have identical amino acid sequences, but slightly different folding. This study opens up a pathway where it would be possible to use photon sources with wavelength that traditionally would not be suitable for imaging, like the AQUA instrument at EuPRAXIA@SPARC_LAB.

Scholarship elegibility

no

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Contribution ID: **8** Type: **Contributed Talk (≈20 minutes)**

Enhanching Radiotherapy with High-Z doped Nitroimidazoles

A way to induce local damage to cancerous tissue is by using radiotherapy-amplifying bioagents doped with high-Z elements. This enables deep core-level ionisation during radiotherapy with X-rays above the K-edge threshold, significantly increasing radiation absorption. Core electron ejection from high-Z elements also triggers a cascade of secondary particles, amplifying damage.
We studied the iodine- and bromine-doped nitroimidazole molecule, an oxygen mimetic that accumulates in oxygen-deficient tumours. We analysed fragmentation mechanisms and radiotherapy-relevant fragments in the gas phase using synchrotron light tuned to K- and L-edges. Additionally, DFT-based molecular dynamics simulations explored bond strengths and fragmentation pathways. To approximate biological conditions, we also examined monosolvated nitroimidazole.
High-Z ionisation produces large quantities of single-atom ions, while C, N, or O 1s-ionization yields heavier fragments like NO2, which can inhibit DNA repair. The addition of a single water molecule affects the local chemical environment and is thus reshaping the dissociation landscape, possibly through hydrogen bonding and charge redistribution—suggested to protect biomolecules from radiation damage.

Scholarship elegibility

no

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Presenter: SVENSSON, Pamela

Contribution ID: **9** Type: **Contributed Talk (≈20 minutes)**

Multidimensional IR Spectroscopy (2D-IR) as tool to study protein dynamics

Ultrafast multidimensional IR spectroscopy (2D-IR) can provide detailed information on local structural dynamics in peptide, proteins or complex systems like models of protein condensates. 2D-IR is a femtosecond laser spectroscopy with its intrinsic time-resolution on par with the fundamental timescale of chemical dynamics, fs to ps. For biological systems the capability to directly probe H-bonding dynamics, changes of electrostatics and conformational dynamics are important. In particular for intrinsically disordered systems or beta-sheet rich structures, 2D-IR has benefits over FTIR spectroscopy, as weak signals (i.e. shoulders) are much sharper in the 2D-IR spectra. The information obtained from 2D-IR spectra is thus complementary to insights from X-Ray diffraction experiments. In this contribution, the basics of 2D-IR and applications to biomolecular systems shall be reviewed and prospects for future integration between 2D-IR and XFEL experiments will be addressed. To this end, we have already performed initial 2D-IR experiments on protein crystals with fixed target sample delivery similar as for TR-SFX experiments.

Scholarship elegibility

no

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Contribution ID: **10** Type: **Contributed Talk (≈20 minutes)**

FTIR (micro-)spectroscopy in situ: Diagnostic Potential and Insights into Amyloid Deposits

Fourier transform infrared (FTIR) (micro-)spectroscopy is a label-free and non-destructive vibrational tool that has been successfully applied to study not only the amyloid structural properties and aggregation mechanisms directly in cells, tissues, or biofluids, but also to gain new insights into the mechanisms of amyloid formation and toxicity[1]. In particular, the use of an infrared microscope allows measuring *in situ* the IR absorption from selected areas of the sample, enabling to explore the colocalization of amyloid deposits with other biomolecules[1].
We employed FTIR microspectroscopy to analyze unfixed human tissues - cardiac and adipose - from patients affected by systemic light chain amyloidosis[2]. We detected the *in situ* marker band of the aggregates, ascribable to amyloid deposits. The possibility to measure unfixed tissue sections made it possible to detect important peculiarities in the spectral features of other biomolecules in cardiac tissues, in areas enriched with aggregates, suggesting a role in particular of lipids in amyloid deposition in vivo[2].
We then applied attenuated total reflection (ATR)-FTIR investigation - coupled to multivariate analysis - to the analysis of adipose tissue aspirates from patients affected by systemic amyloidosis3. We found that the ATR-FTIR approach can differentiate fat aspirates containing amyloid deposits from control specimens with high sensitivity and specificity. Notably, discrimination between amyloid-affected and negative samples was obtained on the basis of the whole spectrum, pointing out that resident lipids are intrinsic features of amyloidosis-affected subcutaneous fat[3].
After our initial studies[2,3], independent groups published works on the potential use of FTIR spectroscopy for the detection and typing of cardiac amyloidosis. The results of subsequent studies[4] confirmed our findings on a larger cohort of patients, emphasizing FTIR spectroscopy as a promising diagnostic method. Here, the scientific background[1,5] and the FTIR spectroscopic approach[1-3] are presented for the detection of cardiac amyloidosis in a clinical setting on the one hand, and for gaining new insights into amyloid deposits *in situ* on the other.

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Scholarship elegibility

no

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Contribution ID: **11** Type: **Flash talk (≈5 minutes)**

TRISS: A Versatile Tool for Unraveling Molecular Mechanisms

TRISS (TRapped Ion Spectrometer Setup) is a novel experimental station at the MAX IV synchrotron facility, designed to investigate fundamental molecular processes relevant to biomolecular and biochemical physics. TRISS uses an electrospray ionization (ESI) source to create ions, which are then fragmented using photons, electrons, or gas. The TRISS setup combines a segmented linear ion trap (the Omnitrap) with time-of-flight mass spectrometry. The Omnitrap's design enables precise manipulation of ions, including their storage, isolation, and fragmentation. By providing detailed insights into how molecular structures break down, TRISS contributes to a deeper understanding of fundamental molecular interactions, with applications in areas such as radiation-induced damage.

Scholarship elegibility

yes

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Presenter: HAFIANI, Ouassim Hocine (Uppsala University)

Contribution ID: **12** Type: **Contributed Talk (≈20 minutes)**

Shedding Light on SARS-CoV-2 viral protein: Infrared Spectroscopy of the Receptor Binding Domain to Spike Protein

Proteins, constituting the virus structure, cover a wide and diverse range of functions. Spike glycoprotein (S) of SARS-CoV-2 is a notable example. As the largest structural protein of the virus, the S protein plays a crucial role in attaching to the host receptor ACE2 through its receptor-binding domain (RBD) [1]. The functionalities of these membrane proteins, such as cellular targeting and recognition, transport, and communication are affected by viral and host factors, including immune evasion, conformational masking of binding domains, glycan shielding, as well as the extent of receptor binding affinity and specificity [1,2].
Understanding the secondary structure of the S protein is crucial for gaining insights into its functionality and into the mechanisms occurring in the viral process, and for addressing specific actions aimed at developing specific drugs, diagnostic tools, and prevention strategies. In this context, vibrational spectroscopy, including infrared (IR) spectroscopy, offers various advantages: it is label-free, fast, non-contact and non-destructive, and it allows multi-component assays. In addition, IR frequency region examines localized molecular vibrations of macromolecules, such as carbohydrates, lipids, DNA and RNA, proteins and their mechanisms of reactions, processes like folding, unfolding, and misfolding, and their secondary structures [3,4].
Here, we present an overview of our results obtained from a systematic and comparative study of SARS-CoV-2 viral protein, its individual protein domains, namely the RBD, S1, S2 regions, and S protein, as well as SARS-CoV-2 S1 variants at serological pH, by measuring the amide I absorption band (1600-1700 cm-1) using Attenuated Total Reflection Infrared (ATR-IR) spectroscopy [5-7]. The combination of experimental results with predictive and computational approaches, such as Define Secondary Structure of Proteins (DSSP) predictions, Molecular Dynamics (MD) simulations and protein Surface Polarity Calculations, provides a comprehensive understanding of the protein domains in terms of their secondary structure content, 3D conformation, and interaction with the solvent.

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Scholarship elegibility

no

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Contribution ID: **13** Type: **Contributed Talk (≈20 minutes)**

Investigating the Origins of Non-Aromatic Fluorescence with Vibrational and X-ray Absorption Spectroscopies

Non-aromatic fluorescence in biomolecules represents a fascinating photophysical phenomenon that challenges conventional understanding of fluorescent mechanisms.. This presentation outlines our ongoing investigation using a combined approach of time-resolved X-ray absorption spectroscopy (TrXAS) and multiple vibrational spectroscopic techniques to explore the fundamental processes governing this phenomenon.

Our research examines L-glutamine (L-glu) and its derivative L-pyroglutamine ammonium (L-pyro-amm), where we hypothesize that hydrogen bonding networks may influence conical intersections (CoIns) and thus modulate nonradiative decay pathways. The complementary techniques of FTIR, far-IR, and Raman spectroscopy are being employed to characterize structural dynamics, while TrXAS measurements at the carbon K-edge at the EIS-TIMEX FEL beamline are anticipated to provide insights into excited-state evolution.

This presentation will discuss our methodological approach, preliminary observations, and the theoretical framework guiding our investigation. We will consider how this integrated spectroscopic strategy may contribute to elucidating the structural and electronic factors that enable non-aromatic fluorescence, with potential implications for the future development of novel fluorescent biomaterials and optical probes.

Scholarship elegibility

no

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Contribution ID: **14** Type: **Contributed Talk (≈20 minutes)**

Molecular dynamics simulations of large gas-phase proteins with the fast multipole method

Classical all-atom molecular dynamics (MD) simulations are a powerful tool for investigating the structures and interactions of biomolecules in the gas phase. Until recently, these simulations were limited to systems containing only a few thousand atoms, due to the quadratic scaling of computational cost with system size. However, the recent integration of a linearly-scaling algorithm for computing the long-range electrostatic forces—the fast multipole method (FMM)—into the MD engine GROMACS has significantly enhanced performance for large biomolecular systems. With this advancement, MD simulations can now be performed efficiently on systems in the megadalton (MDa) range, aligning more closely with the sizes of biomolecules investigated in XFEL experiments.

Here, we demonstrate how to effectively use FMM to achieve high accuracy and performance, and present insights from its initial application to several multimeric protein complexes. Extending the simulation time up to one microsecond, we have gained new insights about the behavior of large proteins in vacuum. Simulations were also performed at multiple temperatures to mimic the effects of thermal activation via collisions with inert gas. These collisions range from low-energy impacts commonly used during electrospray ionization to higher-energy impacts used in techniques like ion mobility spectrometry to probe structural rearrangements and conformational stability. Overall, we demonstrate that FMM-accelerated MD is a powerful tool for investigating large gas-phase biomolecules, yielding results directly relevant to a wide range of gas-phase experimental techniques.

Scholarship elegibility

no

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Contribution ID: **15** Type: **Flash talk (≈5 minutes)**

FEL Coulomb Explosion Imaging: Simulation of Coulomb explosion of highly charged 2-Iodopyridine and comparison to experimental data

X-ray Single Particle Imaging has the aim of imaging biomolecules without the need of crystallization. The invention of X-ray Free Electron Lasers (XFELs) provided the instruments for this imaging process, however the technique is still suffering from low signal to noise ratio. Retrieval of the orientation of the sample in the moment of photon-sample interaction would greatly improve the signal and interpretability of experimental data. During the interaction, the intense radiation of the XFEL leads to high ionization of the sample and to a Coulomb explosion, in which positively charged ions repel each other and fly out of the interaction zone. It was found in recent simulations that a record of the Coulomb explosion doesn't only just retrieve the original orientation of the imaged sample, but also bears structural information itself about the molecule. Hence, it was proposed to explore the relationship between structure and Coulomb explosion, a process called Coulomb Explosion Imaging. The biophysics research group of Uppsala University has developed a Molecular Dynamics/Monte Carlo code called MolDStruct4, which is based on GROMACS. MolDStruct replicates the radiation-induced Coulomb explosion of biomolecules and enables the tracking of ion-trajectories. The code is currently benchmarked against the QM/DFT code SIESTA as well as experimental data to ensure that the simulations of the Coulomb explosions are as realistic as possible. In this process, we investigate the biomolecule 2-Iodopyridine, ionize it up to an average ionization of one per atom and record the Coulomb explosion in simulations with MolDStruct. Then, we compare the results with data from a recent XFEL experiment in which highly ionized 2-Iodopyridine was exploded and the ejected ions were measured using a reaction microscope. Additionally, we execute QM/DFT simulations with the code SIESTA and also record the Coulomb explosion. The simulations with MolDStruct and SIESTA are consistent with one-another and they both replicate well the experimental data. Contrarily to Single Particle Imaging, Coulomb Explosion Imaging does not necessarily need hard X-rays and would be feasible with an intense FEL, such as the one being developed in the EUPRAXIA project. With MolDStruct, the relationship between structural information and Coulomb explosions can be studied intensively in simulations, information which can later on be used to support and enhance experiments on molecular sample structures by adding new imaging possibilities and providing better interpretation of the signal.

Scholarship elegibility

yes

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Contribution ID: **16** Type: **Flash talk (≈5 minutes)**

Brute Force Orientation of Proteins

Diffractive single-particle imaging (SPI) using X-ray free-electron lasers (XFELs) offers a promising approach for determining protein structures without crystallization (Neutze2000) . For successful reconstruction thousands of diffraction images of individual proteins have to be assembled. It has been shown with molecular dynamics simulations that proteins carrying a dipole moment can be oriented with external electric fields (Marklund2017) and that the computer algorithm that sorts the diffraction images benefits from pre-orientation (Marklund2017, Wollter2024). A general estimate of the required minimum field strengths for sufficient orientation is still unknown.\
Expressions for the distribution of the angle θ between the dipole moment μ and the field ϵ were derived for 1) a theoretical mechanical rigid rotor model (RR) of a single protein in which no energy is transferred to inner degrees of freedom and 2) a theoretical thermodynamic model (TM) that assumes equilibration of all internal degrees of freedom in the protein. Molecular dynamics (MD) simulations show similarity with RR for low fields and good agreement with TM for higher fields, when the simulation duration is sufficiently long for the system to reach equilibration.

Based on RR for a single protein and assuming random orientation as well as Boltzmann-distributed rotational kinetic energy when entering the field region, we estimate the distribution of orientation angles for an ensemble of proteins.

To study the beneficial effect of pre-orientation we performed Enhanced EMC (Marklund2017, Wollter2024) with thousands of simulated diffraction pattens (Hantke2016) of proteins oriented according to the theoretical distributions (RR ensemble, TM).

We estimate the required fields for a given dipole moment to achieve given angular confinements and for EEMC to benefit from pre-orientation and relate them to the dipole moments of a dataset of 60k proteins lankar2016).
We conclude that TM is suitable to describe the distribution of angles even for a single protein and that field strengths required to achieve sufficient orientation for EEMC to benefit are technically feasible for a wide range of proteins.

<!— ![Distribution of θ from MD simulations of Ubiquitin. Theoretical distributions of rigid rotor (RR) and the thermodynamic model (TM) are included. The vertical dotted line indicates the starting angle ($\pi/2$) in the simulations. The field varies from 1.0 V/nm (leftmost plot) to 0.001 V/nm (rightmost plot).]()fig:MD

![Required field to achieve $F_\theta(\alpha) = 0.68$ (i.e. angular confinement with 68(dotted) and TM (solid) model. The relative frequencies of dipole moments are shown in the background in blue (a.u.). Within the grey band, EEMC benefit from pre-orientation is greatest. Dipole moments of selected proteins are indicated by their pdb identifier.]()fig:req$_field - -- >$

Scholarship elegibility

no

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Presenter: MANDL, Thomas (Uppsala universitet)

Contribution ID: **17** Type: **Flash talk (≈5 minutes)**

Raman microscopy as a tool to investigate the effects of polystyrene nanoparticle in Zebrafish and human Caco-2 Cells

Marine microplastic pollution has emerged as a major global concern, with growing implications for both marine ecosystems and human health [1]. Polystyrene nanoparticles (PS-NPs) can induce significant biological responses, as demonstrated by combined in vivo and in vitro models. In zebrafish, exposure to PS-NPs resulted in marked changes in eye pigmentation patterns that were not associated with a reduction in melanin content or tyrosinase activity. In this context, Raman microscopy revealed structural differences between treated and untreated samples, possibly related to melanogenesis-inflammatory processes and oxidative stress - an interpretation supported by gene expression data showing strong upregulation of inflammation- and oxidative stress-related markers. In particular, increased expression of rpe65c, a gene associated with retinal health, suggests early signs of retinal dysfunction.
In parallel, human colorectal adenocarcinoma cells (Caco-2), used as an in vitro epithelial model, show efficient internalization of PS-NPs, with Principal Component Analysis (PCA) of Raman mapping data revealing a predominant cytoplasmic and perinuclear localization. Morphological changes consistent with cell death were also observed, indicating a dose- and time-dependent cytotoxic effect. These findings highlight the potential of micro-Raman mapping to reveal the effects of PS-NPs in biological samples, showing their disruptive effects on both developmental and cellular processes, raising concerns about their impact on ocular physiology and epithelial integrity.

Scholarship elegibility

no

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Orienting gas-phase proteins with electric fields for X-ray imaging

Using X-ray diffraction for structure determination is further complicated when the irradiated particles have random and unknown orientations, because it means that the relations between the diffraction images are also unknown. Algorithms exist for recovering the relative orientations between diffraction patterns, but they do not always converge, especially not when faced with scarce or noisy data. Controlling the orientation of the particle would help overcome this problem in single particle imaging and related techniques. We once demonstrated the possibility of orienting proteins in the gas phase without destroying their structures using strong electric fields via the interaction with their electric dipole moments. More recently we have explored more aspects of dipole orientation, including if and how it actually helps the orientation recovery, and how the orientation is affected by a thin layer of water around the protein, which has been shown to have other benefits for single particle imaging. We hope that our results can serve to guide the development of new technology and experiments that utilise dipole orientation for structure determination of macromolecules. To that end, we here present our current research in dipole orientation of gas-phase proteins.

Scholarship elegibility

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Sample delivery for time-resolved studies at the European XFEL

The European XFEL (EuXFEL) enables high resolution and time-resolved structural studies of biological systems. Diffraction, scattering and spectroscopy experiments with a MHz pulse repetition rate, in combination with optical pump-probe or mixing set-ups, give new insights into protein motion and dynamics. To accommodate the MHz repetition rate, sample delivery methods are in demand which ensure quick and efficient sample renewal. The Sample Environment and Characterization (SEC) group at EuXFEL develops these methods and supports users during their experiments. In this presentation sample delivery methods will be discussed and the SEC group activities will be described.

Scholarship elegibility

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