A 32: Interaction with VUV and X-ray Light I (joint session A/MO)

Time: Thursday 14:30–16:30 Location: N 2

Invited Talk A 32.1 Thu 14:30 N 2

IR-laser induced dressing signatures in helium nanodroplets probed by coherent diffractive imaging — •Tom von Scheven, Björn Kruse, and Thomas Fennel — Institute of Physics, University of Rostock, Albert-Einstein-Str. 23-24, D-18059 Rostock, Germany

Single-shot coherent diffractive imaging (CDI) enables the capture of a full diffraction image of a nanostructure using a single flash of XUV or X-ray light. The resulting scattering image encodes both the geometry and the optical properties of the target. So far, this method has mainly been employed for ultrafast structural characterization [1]. However, CDI can also be utilized to resolve ultrafast optical property changes caused by e.g. transient excitation from nonlinear scattering [2], or by illumination with a second ultra-short laser pulse.

Here, we explore the expected signatures for the latter case theoretically, where simultaneous exposure to a strong IR field can induce transient optical properties. To this end, the effective optical properties, emerging from the laser dressing, are extracted from the dipole response of a local quantum description based on an atom-like solution of the time-dependent Schrödinger equation. In a second step, we apply the well-known Mie-solution, to use the obtained optical properties in order to describe the resulting scattering process at helium nanodroplets and compare the results to recent experiments [3].

[1] I. Barke *et al.*, Nat. Commun. **6**, 6187 (2015)
[2] B. Kruse *et al.*, J. Phys.: Photonics **2**, 024007 (2020)
[3] J. Schäfer-Zimmermann *et al.*, arXiv, 2508.19936 (2025)

A 32.2 Thu 15:00 N 2

Non-Hermitian X-Ray photonics and Exceptional Points in thin-film cavities with Mössbauer nuclei — •Fabian Richter[1], Lars Bocklage[2], Sven Velten[2], Ralf Röhlsberger[2], Xiangjin Kong[3], and Adriana Pálffy[1] — [1]Julius-Maximilians-Universität, Würzburg — [2]DESY, Hamburg — [3]Fudan University, Shanghai

Exceptional Points (EPs) mark non-Hermitian degeneracies where eigenvalues and eigenvectors coalesce, producing enhanced sensitivity to perturbations. While widely explored in optical gain-loss systems [1], translating the physics of EPs to the X-ray regime offers distinct advantages such as superior penetration depth, focusability, and detection efficiency.

Here, we investigate non-Hermitian X-ray photonics in thin-film cavities with ^{119}Sn Mössbauer nuclei under grazing-incidence illumination. In addition to theoretical modeling, we analyze experimental time spectra and reflectivity data recorded at PETRA III. The cavity geometry and incidence angle offer tunable control over dissipation [2], while a magnetic hyperfine field enables steering the system toward EPs. In theory, we identify the magnetic field strengths at which EPs emerge and predict qualitatively distinct features in the simulated time spectra. In the experimental time spectra, the situation is more complicated, especially as quadrupole splitting introduces additional spectral structure and increases the complexity of the eigenvalue problem, yet we are able to reliably extract the relevant signatures.

[1] L. Feng et al., Nature Photon. 11, 752-762 (2017).
[2] J. Evers, K. P. Heeg, Phys. Rev. A 88, 043828 (2013).

A 32.3 Thu 15:15 N 2

Single-shot sorting of Mössbauer time-domain data at X-ray free electron lasers — •Miriam Gerharz and Jörg Evers for the Fe-57 EuXFEL-Collaboration — Max-Planck-Institut für Kernphysik, Heidelberg, Germany

Mössbauer spectroscopy is widely used to study structure and dynamics of matter with remarkably high energy resolution, provided by the narrow nuclear resonance line widths. However, the narrow width implies low count rates, such that experiments commonly average over extended measurement times or many x-ray pulses ("shots"). This averaging impedes the study of non-equilibrium phenomena. It has been suggested that X-ray free-electron lasers (XFELs) could enable Mössbauer single-shot measurements without averaging, and a proof-of-principle demonstration has been reported [1]. However, so far, only a tiny fraction of all shots resulted in signal-photon numbers which are sufficiently high for a single-shot analysis. In [2], we develop a sorting approach which allows us to include all data on a single-shot level, independent of the signal content of the individual shots. It utilizes the presence of different dynamics classes, i.e. different nuclear evolutions after each excitation. Each shot is assigned to one of the classes, which can then be analyzed separately. We envision that our approach opens up new grounds for Mössbauer science and beyond, enabling the study of out-of-equilibrium transient dynamics of the nuclei or their environment.

[1] Chumakov et al., Nature Phys 14, 261-264 (2018)
[2] Gerharz et al., arXiv:2509.15833

A 32.4 Thu 15:30 N 2

Neural networks for diffraction image separation — •Nikita Morozov — European XFEL, Schenefeld, Germany

Newly available soft X-ray two-color FEL pulse mode at European XFEL opens a new path to the structural and plasma studies at the nanometer scale. The first pulse, designated as the pump, characterizes the initial state of the object, whereas the second probe pulse captures the system's evolution following its interaction with the pump. The pulses are separated by a short time interval of less than 1 ps. Because this delay is shorter than the detector acquisition time, the state-of-the-art detectors are unable to capture two independent Coherent Diffractive Imaging (CDI) images corresponding to the pump and probe pulses. Instead, it records a single data frame that contains a superposition of CDIs from both FEL pulses, making it almost impossible to follow the evolution process.

This work presents machine learning-based solutions for separating the overlapping components in such data sets. We propose two methods: the first one is based on diffusion probabilistic models, a recent and powerful approach for image generation, and the second using feed-forward convolutional neural networks to solve the same task.

Ideally, after the image separation task is done, the pump and probe densities could be recovered using standard phase retrieval techniques, allowing the excitation-induced changes to be examined in a time-resolved manner.

A 32.5 Thu 15:45 N 2

Laser-driven electron dynamics in helium nanodroplets retrieved from single-shot diffraction patterns — •B. Senfftleben[1,2,3], A. Colombo[1], A. Hoffmann[2], M. Sauppe[1,2], K. Kolatzki[1,2], B. Langbehn[4], J. Schäfer-Zimmermann[1,2], M. Kretschmar[2], M. Krause[2], T. Nagy[2], M. J. J. Vrakking[2], B. Schütte[2], and D. Rupp[1,2] — [1]ETH Zurich, Switzerland — [2]Max-Born-Institut Berlin, Germany — [3]European XFEL, Schenefeld, Germany — [4]TU Berlin, Germany

Coherent diffraction experiments on single particles using intense X-ray or XUV light sources have revolutionized the structural determination of fragile, short-lived nanoscale samples and their dynamics. However, electronic properties are also inherently encoded in the diffraction patterns, but their extraction requires new analysis methods. In our study, we employed a high-harmonic-generation (HHG) light source to perform NIR-XUV pump-probe experiments at photon energies near strong electronic resonances of helium droplets.

In this presentation, several of our analysis approaches to address challenges related to detection artifacts and the multicolor nature of HHG radiation will be discussed. Moreover, initial findings on ultrafast changes in the optical properties and, thus, on electron dynamics of helium nanodroplets will be presented.

A 32.6 Thu 16:00 N 2

Fast Simulation of Wide-Angle Coherent Diffractive Imaging — •Paul Tuemmler, Julia Appertin, Thomas Fennel, and Christian Peltz — Institute of Physics, University of Rostock 18051, Rostock, Germany

Single-shot coherent diffractive imaging with intense XUV and soft X-ray pulses offers the exciting possibility of retrieving both the 3D structure and optical properties of nanoscale objects from a single diffraction pattern. Achieving this, however, requires an accurate description of the underlying wide-angle scattering and propagation effects, which are significantly more complex than in conventional X-ray diffraction.

In this talk, I will introduce the propagation multi-slice Fourier transform method (pMSFT) [1], a fast and accurate approach for simulating the scattering process in this regime. I will outline its derivation from first principles, introduce a unified physical picture to

show its relation to existing methods, and finally present systematic benchmarks demonstrating its superior performance for wide-angle scattering.

[1] P. Tuemmler, et al., Laser Photonics Rev (2025): e02001 https://doi.org/10.1002/lpor.202502001

A 32.7 Thu 16:15 N 2

K-edge core excitation and ionization of singly charged sulfur cations — •Simon Reinwardt[1], Patrick Cieslik[1], Ticia Buhr[2], Alexander Perry-Sassmannshausen[3], Stefan Schippers[3], Alfred Müller[3], Stephan Fritzsche[4,5], Florian Trinter[6], and Michael Martins[1] — [1]Universität Hamburg, Hamburg, Germany — [2]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [3]Justus-Liebig-Universität Gießen, Gießen, Germany — [4]Friedrich-Schiller-Universität Jena, Jena, Germany — [5]Helmholtz-Institut Jena, Jena, Germany — [6]Fritz-Haber-Institut, Berlin, Germany

Near-edge X-ray absorption spectroscopy on sulfur cations provides important reference data for X-ray telescopes and to investigate tender or soft X-ray induced fragmentation processes on sulfur-containing molecular ions. Using the photon-ion merged-beams technique, implemented at the Photon-Ion Spectrometer at PETRA III [1], we measured relative cross sections for twofold, threefold, fourfold, and fivefold photoionization of singly charged sulfur cations in the photon-energy range from 2460 eV to 2510 eV. To theoretically describe the relative cross sections of the different product charge states, we have calculated decay cascades with the Jena Atomic Calculator [2].

[1] S. Schippers *et al.*, J. Phys. B **47**, 115602 (2014).

[2] S. Fritzsche, Comput. Phys. Commun. **240**, 1 (2019).