CPP 30: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods I

Time: Wednesday 16:15–18:30 Location: H34

Invited Talk CPP 30.1 Wed 16:15 H34

Challenges and Opportunities in Bringing Machine Learning to a Synchrotron — •Alexander Hexemer[1], Tanny Chavez[1], Wiebke Köpp[1], Dylan McReynolds[1], Stephan Roth[2], Tim Snow[3], and Sharif Ahmed[3] — [1]Lawrence Berkeley National Lab, Berkeley, CA 94720 — [2]DESY, Hamburg, Germany — [3]Diamond Light Source, Didcot, UK

Artificial intelligence (AI) and machine learning (ML) are transforming scientific research, offering innovative solutions to longstanding data collection, analysis, and interpretation challenges. Synchrotron facilities, which generate vast amounts of complex, high-dimensional data, present unique opportunities to leverage ML to advance materials science. Building on this potential, significant progress is being made at the Advanced Light Source (ALS) to integrate ML tools into various synchrotron applications, including tomography segmentation, autonomous scattering analysis, and multimodal data fusion. Efforts are focused on implementing ML as a service, simplifying adoption by providing web-based solutions designed for seamless use across facilities. These tools aim to enable reliable and scalable ML applications for tasks such as the segmentation of complex 3D tomography datasets and automated experimental feedback in scattering experiments. This talk will explore the evolving role of ML at synchrotrons while addressing key challenges.

CPP 30.2 Wed 16:45 H34

Deep Learning-Driven GISAXS Data Processing for Nanostructure Characterization — •Yufeng Zhai[1], Shachar Dan[1], Julian Heger[2], Peter Müller-Buschbaum[2], and Stephan Roth[1,3] — [1]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Notkestr. 85, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Department of Physics, Chair for Functional Materials, Garching 5, Germany — [3]Royal Institute of Technology (KTH), Stockholm, Sweden

Nanostructured materials, are at the forefront of advanced applications in various fields, owing to their unique physical and chemical properties. Grazing incidence small-angle X-ray scattering (GISAXS) has emerged as a powerful technique for probing the morphology of these nanostructures, offering valuable insights into electron density distributions both at the surface and within thin films. In our approach, we first simulate GISAXS pattern using the Distorted Wave Born Approximation (DWBA) model to generate high-quality training datasets. We then apply deep learning techniques, specifically convolutional neural networks (CNNs), to predict size distributions from GISAXS data. Our results demonstrate that CNNs are highly robust under varying noise conditions and present a promising, time-efficient approach for overcoming the challenges of conventional scattering analysis. This study highlights the potential of integrating advanced computational methods and new analytical tools to enhance the characterization of nanostructures.

CPP 30.3 Wed 17:00 H34

Towards Closing the Autonomous Loop at Multiple Facilities: Developing Web-based User Interfaces and Data Infrastructure for Autonomous Experiments and Automated Data Reduction Workflows — •Benedikt Sochor[1,2], Wiebke Koepp[2], Tanny Chavez[2], Runbo Jiang[2], Dylan McReynolds[2], Marcus Noack[3], Raja Vyshnavi Sriramoju[2], Aidan Coffey[2], Ronald Pandolfi[3], Eric Schaible[2], Chenhui Zhu[2], Frank Schlünzen[1], Stephan V. Roth[1,4], Alexander Hexemer[2], and Sarathlal Koyiloth Vayalil[1,5] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, 6 Cyclotron Rd, Berkeley, 94720, CA, USA — [3]Applied Mathematics and Computational Research Division, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, 94720, CA, USA — [4]KTH Royal Institute of Technology, Teknikringen 56, 100 44 Stockholm, Sweden — [5]UPES, Applied Science Cluster, 248007 Dehradun, India

This project focuses on establishing a robust infrastructure for autonomous scattering experiments at two different synchrotrons: X-ray scattering beamlines at PETRA III (DESY, Hamburg) and at the Advanced Light Source (ALS, Berkeley), initially beamline P03, the micro- and nano-focus small- and wide-angle X-ray scattering beamline (MiNaXS) at DESY, and the SAXS/WAXS/GISAXS/GIWAXS beamline 7.3.3 at the ALS. For selected science cases, the infrastructure's capabilities to handle large datasets during time-resolved and scanning X-ray scattering experiments will be highlighted.

CPP 30.4 Wed 17:15 H34

Imaging techniques for characterization of organic photonic devices utilizing digital luminescence — •Sebastian Kaiser, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden

The generally spin-forbidden T_1-S_0 transition of organic molecules gives access to pronounced long-lived room temperature phosphorescence in surprisingly many molecules, but is easily quenched by environmental oxygen. Controlling and utilizing these competing processes has led to the development of digital luminescence as a photonic design principle and its usage in programmable luminescent tags (PLTs) for application in sensing and information storage. To study and utilize this persistent luminescence, a spatially and temporal resolved imaging technique allows us to extend the characterization of these phenomena beyond spectroscopic measurements. By analyzing high-resolution images, differences in intensity and activation time within a single PLT can be detected, allowing conclusions as to structural irregularities. Evaluating each pixel individually also provides great insight into the statistical distribution of these values without the extensive need for samples and measurements. Thus, imaging techniques offer an excellent extension to the characterization of material systems for digital luminescence and by that allowing us to understand and optimize structure-property relationships. This represents an important step towards the use of PLTs for information storage and exchange.

CPP 30.5 Wed 17:30 H34

3D Nanoprinted Polarization Optics Directly on Optical Fibers — •Tim Stechel — Leibniz Institute of Photonic Technology, Albert-Einstein-Str. 9, 07745 Jena, Germany

Polarization is a fundamental property of electromagnetic radiation, influencing numerous areas of physical sciences and optical technologies. Developing functional interfaces that seamlessly integrate polarization control with fiber optics opens new opportunities for advancing these technologies. Using two-photon polymerization, we fabricate 3D structures on the sub-micron scale, directly on optical fibers. This high-resolution additive manufacturing technique enables the creation of tailored microstructures that can precisely control the polarization state of light as it enters and exits fibers. These custom interfaces are highly adaptable to different fiber types and optical configurations, allowing for enhanced polarization shaping and analysis. In this talk, we present the design process, fabrication process and characterization of the fabricated structures. Our approach combines the versatility of 3D printing with the precision required for nanoscale optical engineering, providing a robust platform for research into light-matter interactions and advancing fiber-based photonic technologies. Potential applications span diverse fields, from telecommunications to advanced optical metrology, demonstrating the broad impact of integrating 3D-printed microstructures with fiber optics.

CPP 30.6 Wed 17:45 H34

Phase-cycling and double-quantum two-dimensional electronic spectroscopy using a common-path birefringent interferometer — Daniel Timmer[1], •Daniel C. Lünemann[1], Moritz Gittinger[1], Antonietta De Sio[1], Cristian Manzoni[2], Giulio Cerullo[2], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität Oldenburg, Germany — [2]Politecnico di Milano, Italy

Ultrafast coherent spectroscopy techniques provide unique insights into the coherent dynamics of atomic, molecular and solid state quantum systems. For this, an experimentally challenging but all the more powerful technique is two-dimensional electronic spectroscopy (2DES), which allows to selectively probe coherent and incoherent couplings and to isolate individual excitation pathways by controlling the absolute phases of the ultrashort optical pulses that interact with the system (phase-cycling, PC). Its experimental implementation can be greatly simplified by employing birefringent in-line interferometers (TWINS) which are inherently phase stable. However, TWINS is so far considered to be incapable of this phase control. Here, we demonstrate PC capabilities for 2DES using an adapted TWINS interferometer by recording rephasing, non-rephasing, zero-quantum and double-quantum 2DES on a molecular J-aggregate. This extension is easy to implement and enables new experimental capabilities for TWINS-based 2DES in multidimensional all-optical and photoemission spectroscopy and microscopy.

[1]: D Timmer, DC Lünemann, et al., Optica (accepted, DOI: 10.1364/OPTICA.543007)

CPP 30.7 Wed 18:00 H34

Real-time structure-transport investigation under mechanical strain in flexible carbon-based conductive polymer nanocomposites — •Sarathlal Koyiloth Vayalil[1,2], Vaishnav B[2], Benedikt Sochor[1], Stephan V. Roth[1,3], Ajay Gupta[2], Tobias Kraus[4,5], and Debmalya Roy[6] — [1]Deutsches Elektronen-Synchrotron DESY, 22607, Hamburg, Germany — [2]Department of Physics, Applied Science cluster, UPES, Dehradun 248007, India — [3]Division of Coating Technology, KTH Royal Institute of Technology, 100 44 Stockholm, Sweden — [4]INM Leibniz-Institute for New Materials, 66123 Saarbruecken, Germany — [5]Colloid and Interface Chemistry, Saarland University, 66123 Saarbruecken, Germany — [6]DMSRDE, Kanpur 208013, India

In this work, an in situ ultra-small angle X-ray scattering combined with electrical transport measurements under mechanical strain has been carried out in flexible, conductive carbon polymer nanocomposite to observe the real-time structural variations in nanofiller morphologies and distribution. For this purpose, the non-polar and polar elastomers viz. polydimethylsiloxane and polyurethane respectively, loaded with 0D Carbon black, 1D Carbon nanotubes, and 2D Graphene has been employed. The study has elucidated that, it is the filler′s fractal dimension that varies rather than aggregate distribution upon stress that decides PNC′s electrical conduction. Further, a novel relationship has been established between fractal dimension and composite′s conductivity, which invincibly guides in designing wearable and flexible conductors.

CPP 30.8 Wed 18:15 H34

In Situ Synchrotron X-Ray Computed Tomography Studies of Specialty Optical Fibers — •Ali Karatutlu[1], Zehra Gizem Mutlay[1], Andriy Budnyk[1], Gianluca Iori[2], Philipp Iori[3], and Bülend Ortaç[1] — [1]Bilkent University, Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM), Ankara, 06800 Turkey — [2]Paul Scherrer Institute PSI Forschungsstrasse 111 5232 Villigen PSI Switzerland — [3]SESAME - Synchrotron-light for Experimental Science and Applications in the Middle East, Allan, 19252, Jordan

Specialty fibers have complex structures due to their geometry, including glass core and cladding, multilayered polymer coatings, and the variations of their elemental compositions. Such complex structures of the specialty and microstructured fibers with air holes and the deformation due to manufacturing fiber lasers during fiber splicing can be investigated by X-ray computed tomography (XCT). The fiber fabrication process includes deposition and post-processes with a subsequent fiber drawing. Here, we present the first official results performed at the station BEATS, SESAME, for the synchrotron XCT imaging of specialty optical fibers all in one, such as polarization-maintaining, active, and photonic crystal fibers. In addition, temperature-dependent XCT measurements provided information on how inner structures, such as polymer coatings, could evolve for PM fibers. The conditions of the XCT measurements and the inner structure of the same type of fibers were found to be crucial and act as the guidelines that will be presented for the structures with sizes close to the voxel size.